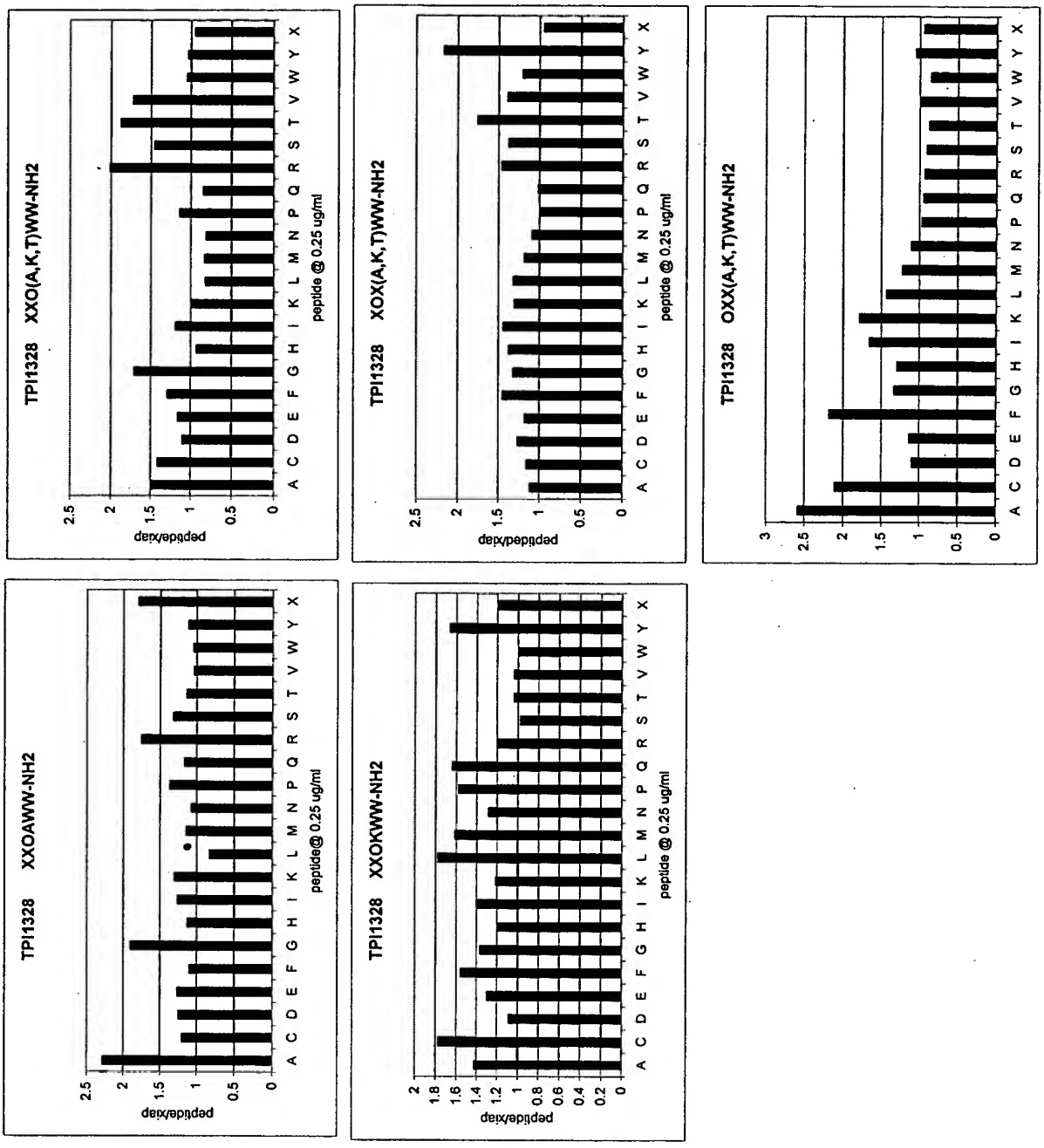


Figure 1

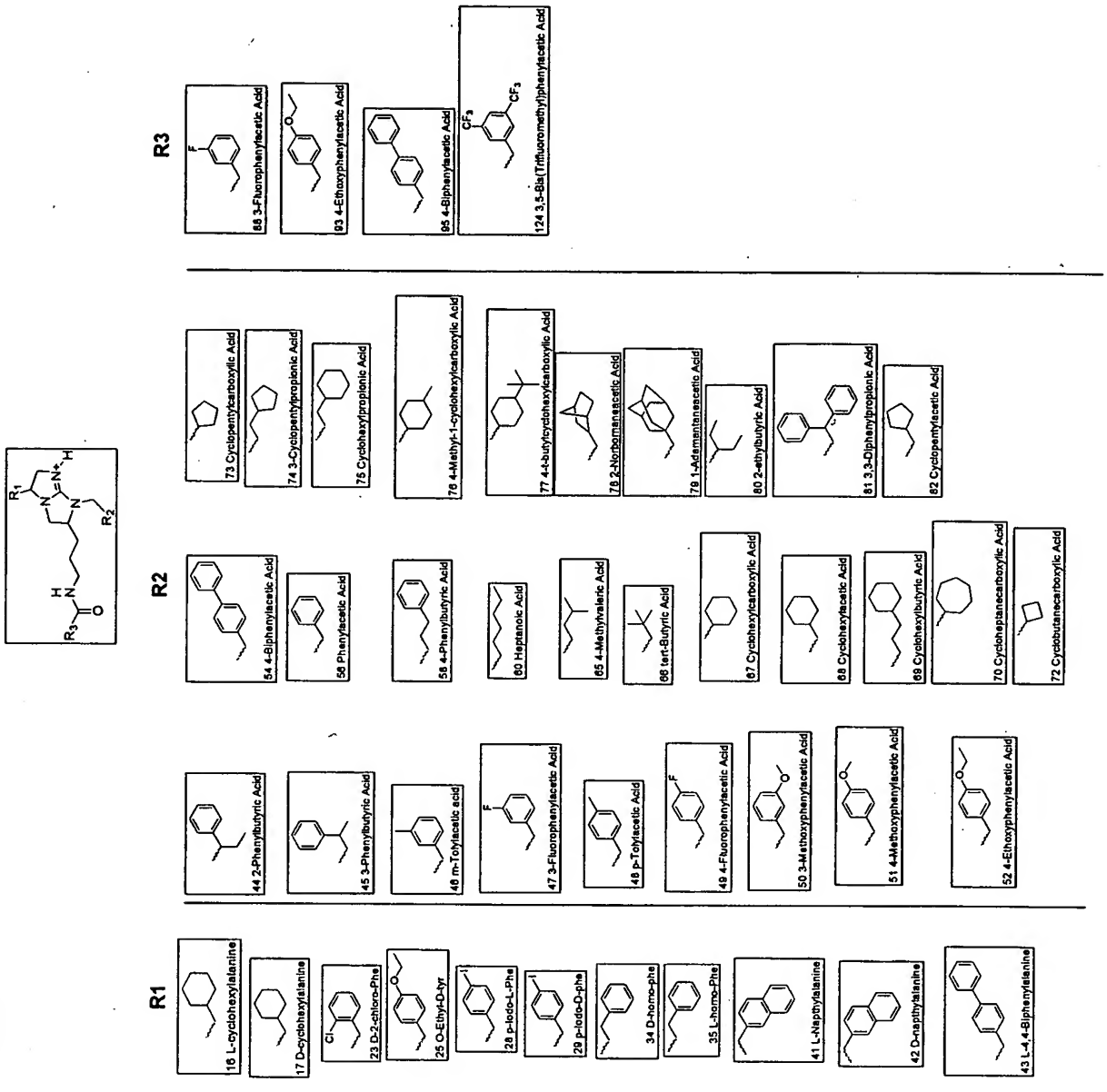
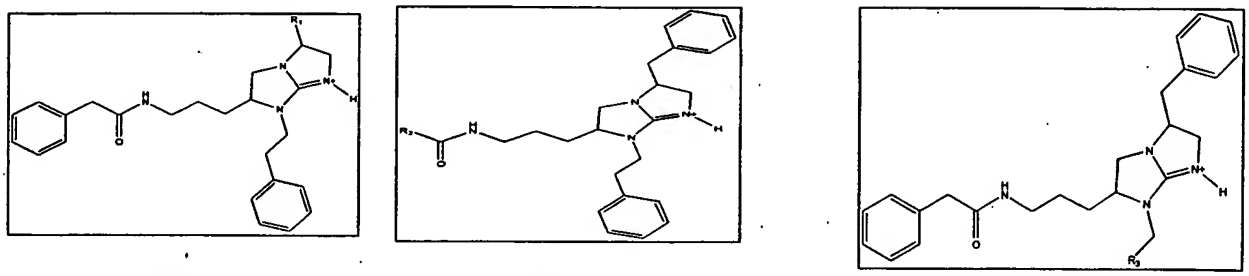


Figure 7
TPI 882

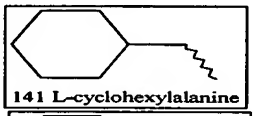
Figure 10

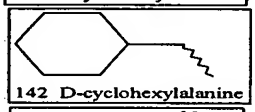
TPI 882 controls

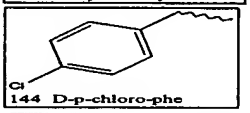
All the compounds below have activity at 8 ug/ml

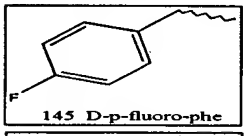


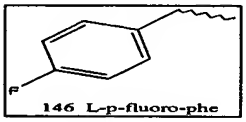
R1

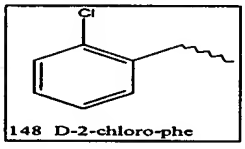

141 L-cyclohexylalanine

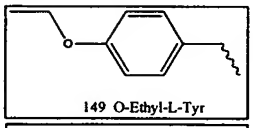

142 D-cyclohexylalanine

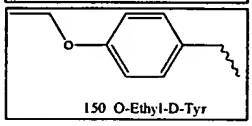

144 D-p-chloro-phe

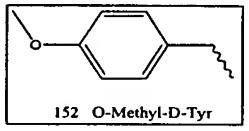

145 D-p-fluoro-phe

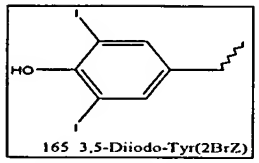

146 L-p-fluoro-phe

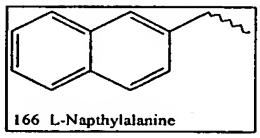

148 D-2-chloro-phe


149 O-Ethyl-L-Tyr

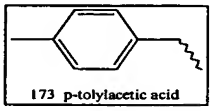

150 O-Ethyl-D-Tyr

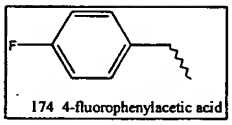

152 O-Methyl-D-Tyr

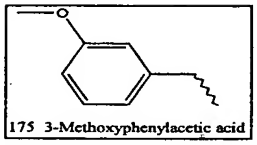

165 3,5-Diiodo-Tyr(2BrZ)

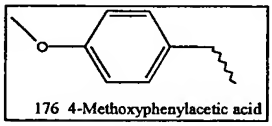

166 L-Napthylalanine

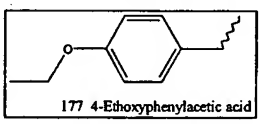
R2

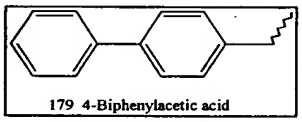

173 p-tolylacetic acid

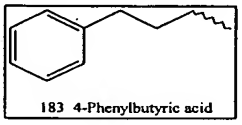

174 4-fluorophenylacetic acid


175 3-Methoxyphenylacetic acid

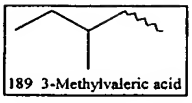

176 4-Methoxyphenylacetic acid

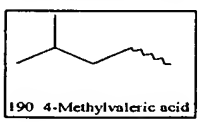

177 4-Ethoxyphenylacetic acid


179 4-Biphenylacetic acid

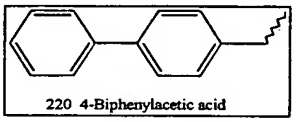

183 4-Phenylbutyric acid


185 Heptanoic acid

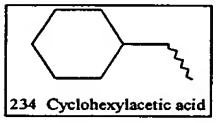

189 3-Methylvaleric acid

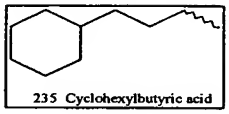

190 4-Methylvaleric acid

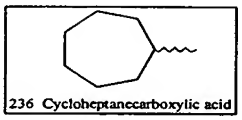
R3

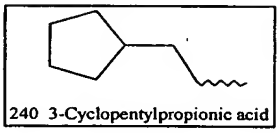

220 4-Biphenylacetic acid

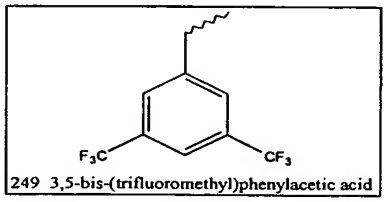

233 Cyclohexanecarboxylic acid


234 Cyclohexylacetic acid


235 Cyclohexylbutyric acid


236 Cycloheptanecarboxylic acid


240 3-Cyclopentylpropionic acid



249 3,5-bis-(trifluoromethyl)phenylacetic acid

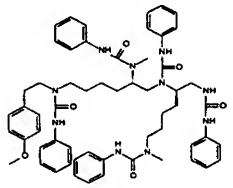
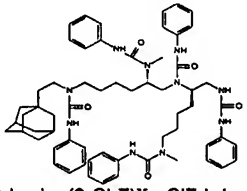
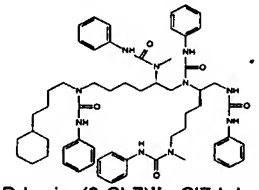
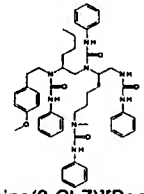
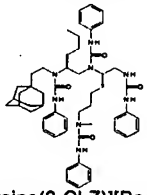
TPI1396	CHEMISTRY	MW	Exact Mass	Name	M Log P	H Bond Acceptor	H Bond Donor	Rule Of Five
1	 [Boc-D-Cyclohexylalanine][a-ClZ-L-Lysine(e-Boc)][1-Adamantaneacetic acid]	1003.3	1002.5	N-[(5R)-6-[(anilinocarbonyl)amino]-5-((anilinocarbonyl){(2S)-6-{(anilinocarbonyl)[2-(4-methoxyphenyl)ethyl]amino}-2-[(anilinocarbonyl)(methyl)amino]hexyl}amino)hexyl]-N-methyl-N'-phenylurea	4.2	16	6	4
2	 [Boc-D-Lysine(2-Cl-Z)][a-ClZ-L-Lysine(e-Boc)][1-Adamantaneacetic acid]	1031.4	1030.6	N-[2-(1-adamantyl)ethyl]-N-{(5S)-6-((anilinocarbonyl){(1R)-1-{[(anilinocarbonyl)amino]methyl}-5-[(anilinocarbonyl)(methyl)amino]pentyl}amino)-5-[(anilinocarbonyl)(methyl)amino]hexyl}-N'-phenylurea	5.1	15	6	4
3	 [Boc-D-Lysine(2-Cl-Z)][a-ClZ-L-Lysine(e-Boc)][Cyclohexanebutyric acid]	1007.3	1006.6	N-[(5R)-6-[(anilinocarbonyl)amino]-5-((anilinocarbonyl){(2S)-6-[(anilinocarbonyl)(4-cyclohexylbutyl)amino]-2-[(anilinocarbonyl)(methyl)amino]hexyl}amino)hexyl]-N-methyl-N'-phenylurea	4.8	15	6	4
4	 [Boc-D-Lysine(2-Cl-Z)][Boc-L-Norleucine][4-Methoxyphenylacetic acid]	855.1	854.5	N-[(5R)-6-[(anilinocarbonyl)amino]-5-[(anilinocarbonyl)((2S)-2-{(anilinocarbonyl)[2-(4-methoxyphenyl)ethyl]amino}hexyl)amino]hexyl}-N-methyl-N'-phenylurea	4.5	13	5	3
5	 [Boc-D-Lysine(2-Cl-Z)][Boc-L-Norleucine][1-Adamantaneacetic acid]	883.2	882.6	N-[2-(1-adamantyl)ethyl]-N-{(1S)-1-{((anilinocarbonyl){(1R)-1-{[(anilinocarbonyl)amino]methyl}-5-[(anilinocarbonyl)(methyl)amino]pentyl}amino)methyl]pentyl}-N'-phenylurea	5.5	12	5	3

Figure 22A

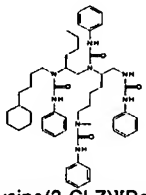
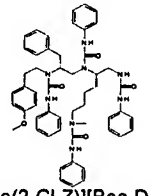
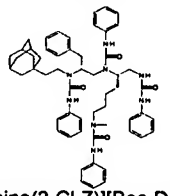
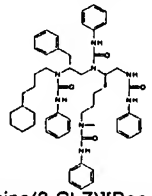
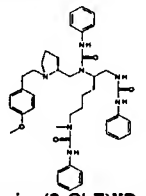
TPI1396	CHEMISTRY	MW	Exact Mass	Name	M Log P	H Bond Acceptor	H Bond Donor	Rule Of Five
6	 [Boc-D-Lysine(2-Cl-Z)][Boc-L-Norleucine][Cyclohexanebutyric acid]	859.2	858.6	N-[(5R)-6-[(anilinocarbonyl)amino]-5-((anilinocarbonyl){(2S)-2-[(anilinocarbonyl)(4-cyclohexylbutyl)amino]hexyl}amino)hexyl]-N-methyl-N'-phenylurea	5.2	12	5	3
7	 [Boc-D-Lysine(2-Cl-Z)][Boc-D-Phenylalanine][4-Methoxyphenylacetic acid]	889.1	888.5	N-[(5R)-6-[(anilinocarbonyl)amino]-5-[(anilinocarbonyl)((2R)-2-{(anilinocarbonyl)[2-(4-methoxyphenyl)ethyl]amino}-3-phenylpropyl)amino]hexyl]-N-methyl-N'-phenylurea	4.8	13	5	3
8	 [Boc-D-Lysine(2-Cl-Z)][Boc-D-Phenylalanine][1-Adamantaneacetic acid]	917.2	916.5	N-[2-(1-adamantyl)ethyl]-N-[(1R)-2-((anilinocarbonyl){(1R)-1-{[(anilinocarbonyl)amino]methyl}-5-[(anilinocarbonyl)(methyl)amino]pentyl}amino)-1-benzylethyl]-N'-phenylurea	5.8	12	5	3
9	 [Boc-D-Lysine(2-Cl-Z)][Boc-D-Phenylalanine][Cyclohexanebutyric acid]	893.2	892.5	N-[(5R)-6-[(anilinocarbonyl)amino]-5-((anilinocarbonyl){(2R)-2-[(anilinocarbonyl)(4-cyclohexylbutyl)amino]-3-phenylpropyl}amino)hexyl]-N-methyl-N'-phenylurea	5.5	12	5	3
10	 [Boc-D-Lysine(2-Cl-Z)][Boc-L-Proline][4-Methoxyphenylacetic acid]	719.9	719.4	N-{(5R)-6-[(anilinocarbonyl)amino]-5-[(anilinocarbonyl)(((2S)-1-[2-(4-methoxyphenyl)ethyl]pyrrolidin-2-yl)methyl)amino]hexyl}-N-methyl-N'-phenylurea	3.7	11	4	2

Figure 22A (cont.)

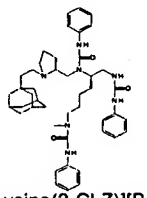
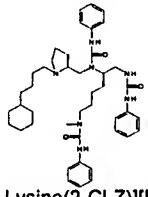
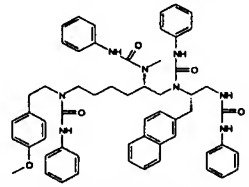
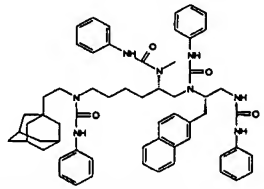
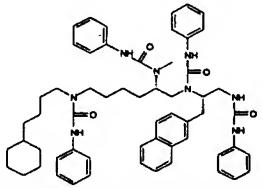
TPI1396	CHEMISTRY	MW	Exact Mass	Name	M Log P	H Bond Acceptor	H Bond Donor	Rule Of Five
11	 [Boc-D-Lysine(2-Cl-Z)][Boc-L-Proline][1-Adamantaneacetic acid]	748.0	747.5	N-(((2S)-1-[2-(1-adamantyl)ethyl]pyrrolidin-2-yl}methyl)-N-{(1R)-1-{[(anilinocarbonyl)amino]methyl}-5-[(anilinocarbonyl)(methyl)amino]pentyl}-N'-phenylurea	4.9	10	4	2
12	 [Boc-D-Lysine(2-Cl-Z)][Boc-L-Proline][Cyclohexanebutyric acid]	724.0	723.5	N-[(5R)-6-[(anilinocarbonyl)amino]-5-((anilinocarbonyl){[(2S)-1-(4-cyclohexylbutyl)pyrrolidin-2-yl]methyl}amino)hexyl]-N-methyl-N'-phenylurea	4.6	10	4	2
13	 [Boc-L-3-(2-Naphthyl)-Alanine][a-ClZ-L-Lysine(e-Boc)][4-Methoxyphenylacetic acid]	939.2	938.5	N-[(1S)-2-[(anilinocarbonyl)amino]-1-(2-naphthylmethyl)ethyl]-N-{(2S)-6-{(anilinocarbonyl)[2-(4-methoxyphenyl)ethyl]amino}-2-[(anilinocarbonyl)(methyl)amino]hexyl}-N'-phenylurea	5.2	13	5	3
14	 [Boc-L-3-(2-Naphthyl)-Alanine][a-ClZ-L-Lysine(e-Boc)][1-Adamantaneacetic acid]	967.3	966.6	N-[2-(1-adamantyl)ethyl]-N-{(5S)-6-{(anilinocarbonyl)[(1S)-2-[(anilinocarbonyl)amino]-1-(2-naphthylmethyl)ethyl]amino}-5-[(anilinocarbonyl)(methyl)amino]hexyl}-N'-phenylurea	6.2	12	5	3
15	 [Boc-L-3-(2-Naphthyl)-Alanine][a-ClZ-L-Lysine(e-Boc)][Cyclohexanebutyric acid]	943.2	942.6	N-[(1S)-2-[(anilinocarbonyl)amino]-1-(2-naphthylmethyl)ethyl]-N-{(2S)-6-[(anilinocarbonyl)(4-cyclohexylbutyl)amino]-2-[(anilinocarbonyl)(methyl)amino]hexyl}-N'-phenylurea	5.9	12	5	3

Figure 22A (cont.)

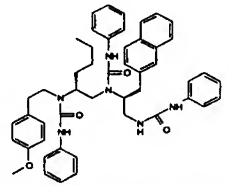
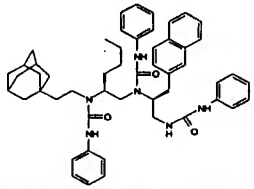
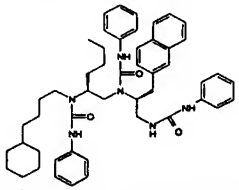
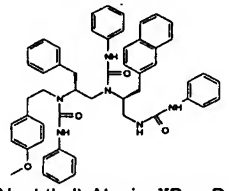
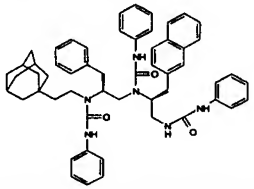
TPI1396	CHEMISTRY	MW	Exact Mass	Name	M Log P	H Bond Acceptor	H Bond Donor	Rule Of Five
16	 [Boc-L-3-(2-Naphthyl)-Alanine][Boc-L-Norleucine][4-Methoxyphenylacetic acid]	791.0	790.4	N-[(1S)-2-[(anilinocarbonyl)amino]-1-(2-naphthylmethyl)ethyl]-N-((2S)-2-{(anilinocarbonyl)[2-(4-methoxyphenyl)ethyl]amino}hexyl)-N'-phenylurea	5.6	10	4	2
17	 [Boc-L-3-(2-Naphthyl)-Alanine][Boc-L-Norleucine][1-Adamantaneacetic acid]	819.1	818.5	N-[2-(1-adamantyl)ethyl]-N-[(1S)-1-({(anilinocarbonyl)[(1S)-2-[(anilinocarbonyl)amino]-1-(2-naphthylmethyl)ethyl]amino}methyl)pentyl]-N'-phenylurea	6.3	9	4	2
18	 [Boc-L-3-(2-Naphthyl)-Alanine][Boc-L-Norleucine][Cyclohexanebutyric acid]	795.1	794.5	N-[(1S)-2-[(anilinocarbonyl)amino]-1-(2-naphthylmethyl)ethyl]-N-((2S)-2-[(anilinocarbonyl)(4-cyclohexylbutyl)amino]hexyl)-N'-phenylurea	6.0	9	4	2
19	 [Boc-L-3-(2-Naphthyl)-Alanine][Boc-D-Phenylalanine][4-Methoxyphenylacetic acid]	825.0	824.4	N-[(1S)-2-[(anilinocarbonyl)amino]-1-(2-naphthylmethyl)ethyl]-N-((2S)-2-{(anilinocarbonyl)[2-(4-methoxyphenyl)ethyl]amino}-3-phenylpropyl)-N'-phenylurea	5.9	10	4	2
20	 [Boc-L-3-(2-Naphthyl)-Alanine][Boc-D-Phenylalanine][1-Adamantaneacetic acid]	853.1	852.5	N-[2-(1-adamantyl)ethyl]-N-((1S)-2-{(anilinocarbonyl)[(1S)-2-[(anilinocarbonyl)amino]-1-(2-naphthylmethyl)ethyl]amino}-1-benzylethyl)-N'-phenylurea	6.6	9	4	2

Figure 22A (cont.)

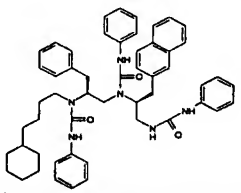
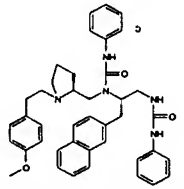
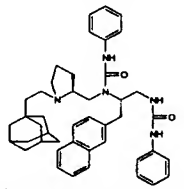
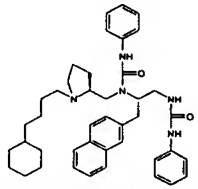
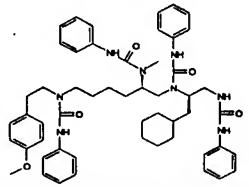
TPI1396	CHEMISTRY	MW	Exact Mass	Name	M Log P	H Bond Acceptor	H Bond Donor	Rule Of Five
21	 [Boc-L-3-(2-Naphthyl)-Alanine][Boc-D-Phenylalanine][Cyclohexanebutyric acid]	829.1	828.5	N-[(1S)-2-[(anilinocarbonyl)amino]-1-(2-naphthylmethyl)ethyl]-N-{(2S)-2-[(anilinocarbonyl)(4-cyclohexylbutyl)amino]-3-phenylpropyl}-N'-phenylurea	6.3	9	4	2
22	 [Boc-L-3-(2-Naphthyl)-Alanine][Boc-L-Proline][4-Methoxyphenylacetic acid]	655.8	655.4	N-[(1S)-2-[(anilinocarbonyl)amino]-1-(2-naphthylmethyl)ethyl]-N-({(2S)-1-[2-(4-methoxyphenyl)ethyl]pyrrolidin-2-yl}methyl)-N'-phenylurea	4.6	8	3	2
23	 [Boc-L-3-(2-Naphthyl)-Alanine][Boc-L-Proline][1-Adamantaneacetic acid]	683.9	683.4	N-({(2S)-1-[2-(1-adamantyl)ethyl]pyrrolidin-2-yl}methyl)-N-[(1S)-2-[(anilinocarbonyl)amino]-1-(2-naphthylmethyl)ethyl]-N'-phenylurea	5.8	7	3	2
24	 [Boc-L-3-(2-Naphthyl)-Alanine][Boc-L-Proline][Cyclohexanebutyric acid]	659.9	659.4	N-[(1S)-2-[(anilinocarbonyl)amino]-1-(2-naphthylmethyl)ethyl]-N-{[(2S)-1-(4-cyclohexylbutyl)pyrrolidin-2-yl]methyl}-N'-phenylurea	5.4	7	3	2
25	 [Boc-D-Cyclohexylalanine][a-CIZ-L-Lysine(e-Boc)][4-Methoxyphenylacetic acid]	895.2	894.5	N-[(1R)-2-[(anilinocarbonyl)amino]-1-(cyclohexylmethyl)ethyl]-N-{(2S)-6-{(anilinocarbonyl)[2-(4-methoxyphenyl)ethyl]amino}-2-[(anilinocarbonyl)(methyl)amino]hexyl}-N'-phenylurea	4.6	13	5	3

Figure 22A (cont.)

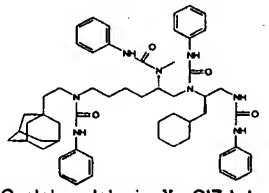
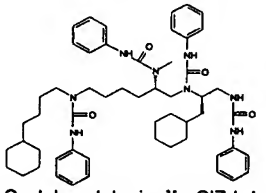
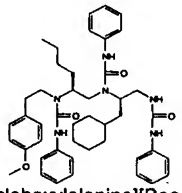
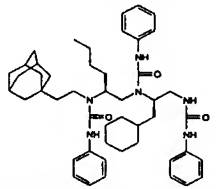
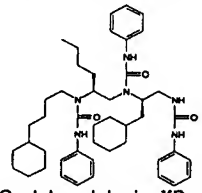
TPI1396	CHEMISTRY	MW	Exact Mass	Name	M Log P	H Bond Acceptor	H Bond Donor	Rule Of Five
26	 [Boc-D-Cyclohexylalanine][a-ClZ-L-Lysine(e-Boc)][1-Adamantaneacetic acid]	923.3	922.6	N-[2-(1-adamantyl)ethyl]-N-{(5S)-6-{(anilinocarbonyl)[(1R)-2-[(anilinocarbonyl)amino]-1-(cyclohexylmethyl)ethyl]amino}-5-[(anilinocarbonyl)(methyl)amino]hexyl}-N'-phenylurea	6.0	12	5	3
27	 [Boc-D-Cyclohexylalanine][a-ClZ-L-Lysine(e-Boc)][Cyclohexanebutyric acid]	899.2	898.6	N-[(1R)-2-[(anilinocarbonyl)amino]-1-(cyclohexylmethyl)ethyl]-N-{(2S)-6-[(anilinocarbonyl)(4-cyclohexylbutyl)amino]-2-[(anilinocarbonyl)(methyl)amino]hexyl}-N'-phenylurea	5.7	12	5	3
28	 [Boc-D-Cyclohexylalanine][Boc-L-Norleucine][4-Methoxyphenylacetic acid]	747.0	746.5	N-[(1R)-2-[(anilinocarbonyl)amino]-1-(cyclohexylmethyl)ethyl]-N-((2S)-2-{(anilinocarbonyl)[2-(4-methoxyphenyl)ethyl]amino}hexyl)-N'-phenylurea	4.9	10	4	2
29	 [Boc-D-Cyclohexylalanine][Boc-L-Norleucine][1-Adamantaneacetic acid]	775.1	774.5	N-[2-(1-adamantyl)ethyl]-N-[(1S)-1-({(anilinocarbonyl)[(1R)-2-[(anilinocarbonyl)amino]-1-(cyclohexylmethyl)ethyl]amino}methyl)pentyl]-N'-phenylurea	6.1	9	4	2
30	 [Boc-D-Cyclohexylalanine][Boc-L-Norleucine][Cyclohexanebutyric acid]	751.1	750.5	N-[(1R)-2-[(anilinocarbonyl)amino]-1-(cyclohexylmethyl)ethyl]-N-{(2S)-2-[(anilinocarbonyl)(4-cyclohexylbutyl)amino]hexyl}-N'-phenylurea	5.8	9	4	2

Figure 22A (cont.)

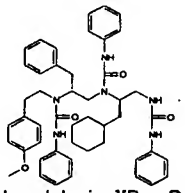
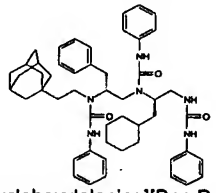
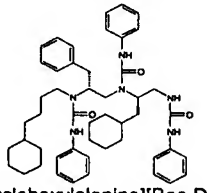
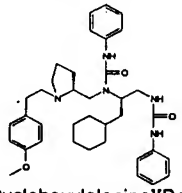
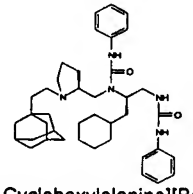
TPI1396	CHEMISTRY	MW	Exact Mass	Name	M Log P	H Bond Acceptor	H Bond Donor	Rule Of Five
31	 [Boc-D-Cyclohexylalanine][Boc-D-Phenylalanine][4-Methoxyphenylacetic acid]	781.0	780.4	N-[(1R)-2-[(anilinocarbonyl)amino]-1-(cyclohexylmethyl)ethyl]-N-((2R)-2-{(anilinocarbonyl)[2-(4-methoxyphenyl)ethyl]amino}-3-phenylpropyl)-N'-phenylurea	5.2	10	4	2
32	 [Boc-D-Cyclohexylalanine][Boc-D-Phenylalanine][1-Adamantaneacetic acid]	809.1	808.5	N-[2-(1-adamantyl)ethyl]-N-((1R)-2-{(anilinocarbonyl)[(1R)-2-[(anilinocarbonyl)amino]-1-(cyclohexylmethyl)ethyl]amino}-1-benzylethyl)-N'-phenylurea	6.4	9	4	2
33	 [Boc-D-Cyclohexylalanine][Boc-D-Phenylalanine][Cyclohexanebutyric acid]	785.1	784.5	N-[(1R)-2-[(anilinocarbonyl)amino]-1-(cyclohexylmethyl)ethyl]-N-((2R)-2-[(anilinocarbonyl)(4-cyclohexylbutyl)amino]-3-phenylpropyl)-N'-phenylurea	6.0	9	4	2
34	 [Boc-D-Cyclohexylalanine][Boc-L-Proline][4-Methoxyphenylacetic acid]	611.8	611.4	N-[(1R)-2-[(anilinocarbonyl)amino]-1-(cyclohexylmethyl)ethyl]-N-({(2S)-1-[2-(4-methoxyphenyl)ethyl]pyrrolidin-2-yl}methyl)-N'-phenylurea	4.3	8	3	2
35	 [Boc-D-Cyclohexylalanine][Boc-L-Proline][1-Adamantaneacetic acid]	639.9	639.5	N-({(2S)-1-[2-(1-adamantyl)ethyl]pyrrolidin-2-yl}methyl)-N-[(1R)-2-[(anilinocarbonyl)amino]-1-(cyclohexylmethyl)ethyl]-N'-phenylurea	5.5	7	3	2

Figure 22A (cont.)

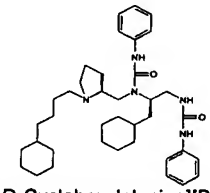
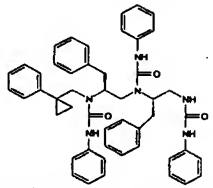
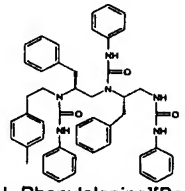
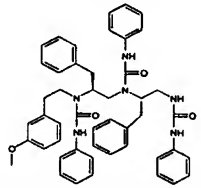
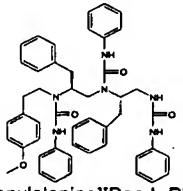
TPI1396	CHEMISTRY	MW	Exact Mass	Name	M Log P	H Bond Acceptor	H Bond Donor	Rule Of Five
36	 [Boc-D-Cyclohexylalanine][Boc-L-Proline][Cyclohexanebutyric acid]	615.9	615.5	N-[(1R)-2-[(anilinocarbonyl)amino]-1-(cyclohexylmethyl)ethyl]-N-[[(2S)-1-(4-cyclohexylbutyl)pyrrolidin-2-yl]methyl]-N'-phenylurea	5.1	7	3	2
37	 [Boc-L-Phenylalanine][Boc-L-Phenylalanine][1-Phenyl-1-Cyclopropanecarboxylic acid]	771.0	770.4	N-{(1S)-2-[(anilinocarbonyl)amino]-1-benzylethyl}-N-((2S)-2-{(anilinocarbonyl)[(1-phenylcyclopropyl)methyl]amino}-3-phenylpropyl)-N'-phenylurea	5.7	9	4	2
38	 [Boc-L-Phenylalanine][Boc-L-Phenylalanine][p-Tolylacetic acid]	759.0	758.4	N-{(1S)-2-[(anilinocarbonyl)amino]-1-benzylethyl}-N-((2S)-2-{(anilinocarbonyl)[2-(4-methylphenyl)ethyl]amino}-3-phenylpropyl)-N'-phenylurea	5.9	9	4	2
39	 [Boc-L-Phenylalanine][Boc-L-Phenylalanine][3-Methoxyphenylacetic acid]	775.0	774.4	N-{(1S)-2-[(anilinocarbonyl)amino]-1-benzylethyl}-N-((2S)-2-{(anilinocarbonyl)[2-(3-methoxyphenyl)ethyl]amino}-3-phenylpropyl)-N'-phenylurea	5.4	10	4	2
40	 [Boc-L-Phenylalanine][Boc-L-Phenylalanine][4-Methoxyphenylacetic acid]	775.0	774.4	N-{(1S)-2-[(anilinocarbonyl)amino]-1-benzylethyl}-N-((2S)-2-{(anilinocarbonyl)[2-(4-methoxyphenyl)ethyl]amino}-3-phenylpropyl)-N'-phenylurea	5.4	10	4	2

Figure 22A (cont.)

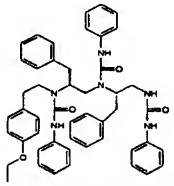
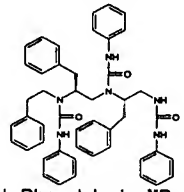
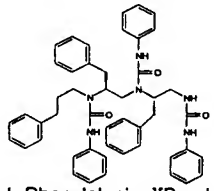
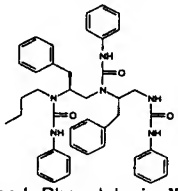
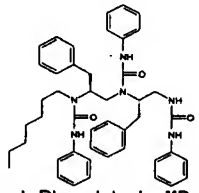
TPI1396	CHEMISTRY	MW	Exact Mass	Name	M Log P	H Bond Acceptor	H Bond Donor	Rule Of Five
41	 [Boc-L-Phenylalanine][Boc-L-Phenylalanine][4-Ethoxyphenylacetic acid]	789.0	788.4	N-{(1S)-2-[(anilinocarbonyl)amino]-1-benzylethyl}-N-((2S)-2-{(anilinocarbonyl)[2-(4-ethoxyphenyl)ethyl]amino}-3-phenylpropyl)-N'-phenylurea	5.6	10	4	2
42	 [Boc-L-Phenylalanine][Boc-L-Phenylalanine][Phenylacetic acid]	744.9	744.4	N-{(1S)-2-[(anilinocarbonyl)amino]-1-benzylethyl}-N-{(2S)-2-[(anilinocarbonyl)(2-phenylethyl)amino]-3-phenylpropyl}-N'-phenylurea	5.7	9	4	2
43	 [Boc-L-Phenylalanine][Boc-L-Phenylalanine][Hydrocinnamic acid]	759.0	758.4	N-{(1S)-2-[(anilinocarbonyl)amino]-1-benzylethyl}-N-{(2S)-2-[(anilinocarbonyl)(3-phenylpropyl)amino]-3-phenylpropyl}-N'-phenylurea	5.9	9	4	2
44	 [Boc-L-Phenylalanine][Boc-L-Phenylalanine][Butyric acid]	696.9	696.4	N-{(1S)-2-[(anilinocarbonyl)amino]-1-benzylethyl}-N-{(2S)-2-[(anilinocarbonyl)(butyl)amino]-3-phenylpropyl}-N'-phenylurea	5.3	9	4	2
45	 [Boc-L-Phenylalanine][Boc-L-Phenylalanine][Heptanoic acid]	739.0	738.4	N-{(1S)-2-[(anilinocarbonyl)amino]-1-benzylethyl}-N-{(2S)-2-[(anilinocarbonyl)(heptyl)amino]-3-phenylpropyl}-N'-phenylurea	5.8	9	4	2

Figure 22A (cont.)

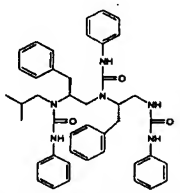
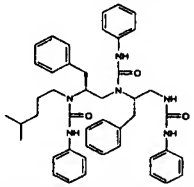
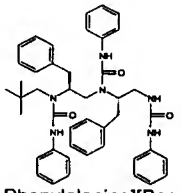
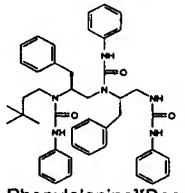
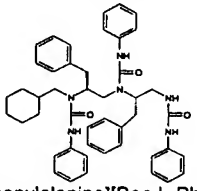
TPI1396	CHEMISTRY	MW	Exact Mass	Name	M Log P	H Bond Acceptor	H Bond Donor	Rule Of Five
46	 [Boc-L-Phenylalanine][Boc-L-Phenylalanine][Isobutyric acid]	696.9	696.4	N-{(1S)-2-[(anilinocarbonyl)amino]-1-benzylethyl}-N-{(2S)-2-[(anilinocarbonyl)(isobutyl)amino]-3-phenylpropyl}-N'-phenylurea	5.3	9	4	2
47	 [Boc-L-Phenylalanine][Boc-L-Phenylalanine][4-Methylvaleric acid]	724.9	724.4	N-{(1S)-2-[(anilinocarbonyl)amino]-1-benzylethyl}-N-{(2S)-2-[(anilinocarbonyl)(4-methylpentyl)amino]-3-phenylpropyl}-N'-phenylurea	5.6	9	4	2
48	 [Boc-L-Phenylalanine][Boc-L-Phenylalanine][Trimethylacetic acid]	710.9	710.4	N-{(1S)-2-[(anilinocarbonyl)amino]-1-benzylethyl}-N-{(2S)-2-[(anilinocarbonyl)(neopentyl)amino]-3-phenylpropyl}-N'-phenylurea	5.4	9	4	2
49	 [Boc-L-Phenylalanine][Boc-L-Phenylalanine][tert-Butylacetic acid]	724.9	724.4	N-{(1S)-2-[(anilinocarbonyl)amino]-1-benzylethyl}-N-{(2S)-2-[(anilinocarbonyl)(3,3-dimethylbutyl)amino]-3-phenylpropyl}-N'-phenylurea	5.6	9	4	2
50	 [Boc-L-Phenylalanine][Boc-L-Phenylalanine][Cyclohexanecarboxylic acid]	737.0	736.4	N-{(1S)-2-[(anilinocarbonyl)amino]-1-benzylethyl}-N-{(2S)-2-[(anilinocarbonyl)(cyclohexylmethyl)amino]-3-phenylpropyl}-N'-phenylurea	5.4	9	4	2

Figure 22A (cont.)

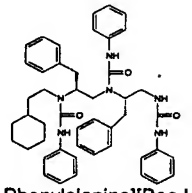
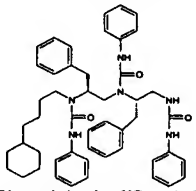
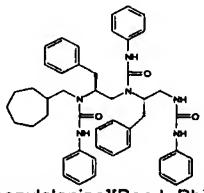
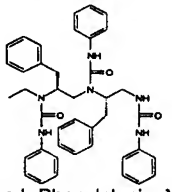
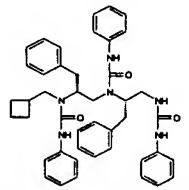
TPI1396	CHEMISTRY	MW	Exact Mass	Name	M Log P	H Bond Acceptor	H Bond Donor	Rule Of Five
51	 [Boc-L-Phenylalanine][Boc-L-Phenylalanine][Cyclohexylacetic acid]	751.0	750.4	N-{(1S)-2-[(anilinocarbonyl)amino]-1-benzylethyl}-N-{(2S)-2-[(anilinocarbonyl)(2-cyclohexylethyl)amino]-3-phenylpropyl}-N'-phenylurea	5.5	9	4	2
52	 [Boc-L-Phenylalanine][Boc-L-Phenylalanine][Cyclohexanebutyric acid]	779.0	778.5	N-{(1S)-2-[(anilinocarbonyl)amino]-1-benzylethyl}-N-{(2S)-2-[(anilinocarbonyl)(4-cyclohexylbutyl)amino]-3-phenylpropyl}-N'-phenylurea	5.8	9	4	2
53	 [Boc-L-Phenylalanine][Boc-L-Phenylalanine][Cycloheptanecarboxylic acid]	751.0	750.4	N-{(1S)-2-[(anilinocarbonyl)amino]-1-benzylethyl}-N-{(2S)-2-[(anilinocarbonyl)(cycloheptylmethyl)amino]-3-phenylpropyl}-N'-phenylurea	5.5	9	4	2
54	 [Boc-L-Phenylalanine][Boc-L-Phenylalanine][Acetic acid]	668.8	668.3	N-{(1S)-2-[(anilinocarbonyl)amino]-1-benzylethyl}-N-{(2S)-2-[(anilinocarbonyl)(ethyl)amino]-3-phenylpropyl}-N'-phenylurea	4.9	9	4	2
55	 [Boc-L-Phenylalanine][Boc-L-Phenylalanine][Cyclobutanecarboxylic acid]	708.9	708.4	N-{(1S)-2-[(anilinocarbonyl)amino]-1-benzylethyl}-N-{(2S)-2-[(anilinocarbonyl)(cyclobutylmethyl)amino]-3-phenylpropyl}-N'-phenylurea	5.0	9	4	2

Figure 22A (cont.)

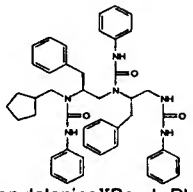
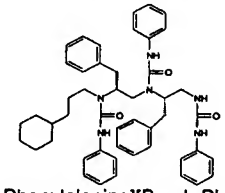
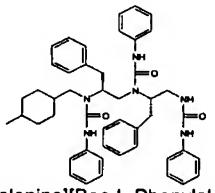
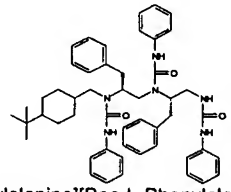
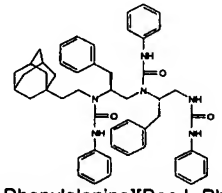
TPI1396	CHEMISTRY	MW	Exact Mass	Name	M Log P	H Bond Acceptor	H Bond Donor	Rule Of Five
56	 [Boc-L-Phenylalanine][Boc-L-Phenylalanine][Cyclopentanecarboxylic acid]	722.9	722.4	N-{(1S)-2-[(anilinocarbonyl)amino]-1-benzylethyl}-N-{(2S)-2-[(anilinocarbonyl)(cyclopentylmethyl)amino]-3-phenylpropyl}-N'-phenylurea	5.2	9	4	2
57	 [Boc-L-Phenylalanine][Boc-L-Phenylalanine][Cyclohexanepropionic acid]	765.0	764.4	N-{(1S)-2-[(anilinocarbonyl)amino]-1-benzylethyl}-N-{(2S)-2-[(anilinocarbonyl)(3-cyclohexylpropyl)amino]-3-phenylpropyl}-N'-phenylurea	5.7	9	4	2
58	 [Boc-L-Phenylalanine][Boc-L-Phenylalanine][4-Methyl-1-cyclohexanecarboxylic acid]	751.0	750.4	N-{(1S)-2-[(anilinocarbonyl)amino]-1-benzylethyl}-N-{(2S)-2-{(anilinocarbonyl)[(4-methylcyclohexyl)methyl]amino}-3-phenylpropyl}-N'-phenylurea	5.5	9	4	2
59	 [Boc-L-Phenylalanine][Boc-L-Phenylalanine][4-tert-Butyl-cyclohexanecarboxylic acid]	793.1	792.5	N-{(1S)-2-[(anilinocarbonyl)amino]-1-benzylethyl}-N-{(2S)-2-{(anilinocarbonyl)[(4-tert-butylcyclohexyl)methyl]amino}-3-phenylpropyl}-N'-phenylurea	6.0	9	4	2
60	 [Boc-L-Phenylalanine][Boc-L-Phenylalanine][1-Adamantaneacetic acid]	803.1	802.5	N-[2-(1-adamantyl)ethyl]-N-[(1S)-2-((anilinocarbonyl){(1S)-2-[(anilinocarbonyl)amino]-1-benzylethyl}amino)-1-benzylethyl]-N'-phenylurea	6.2	9	4	2

Figure 22A (cont.)

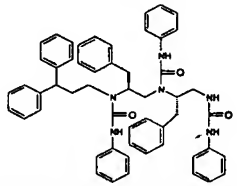
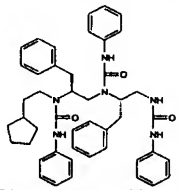
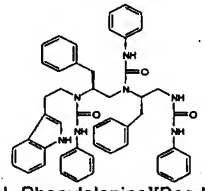
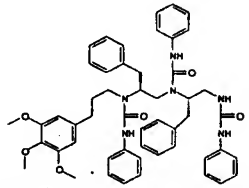
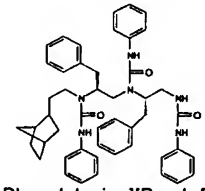
TPI1396	CHEMISTRY	MW	Exact Mass	Name	M Log P	H Bond Acceptor	H Bond Donor	Rule Of Five
61	 [Boc-L-Phenylalanine][Boc-L-Phenylalanine][3,3-Diphenylpropionic acid]	835.1	834.4	N-{(1S)-2-[(anilinocarbonyl)amino]-1-benzylethyl}-N-{(2S)-2-[(anilinocarbonyl)(3,3-diphenylpropyl)amino]-3-phenylpropyl}-N'-phenylurea	6.6	9	4	2
62	 [Boc-L-Phenylalanine][Boc-L-Phenylalanine][Cyclopentylacetic acid]	737.0	736.4	N-{(1S)-2-[(anilinocarbonyl)amino]-1-benzylethyl}-N-{(2S)-2-[(anilinocarbonyl)(2-cyclopentylethyl)amino]-3-phenylpropyl}-N'-phenylurea	5.4	9	4	2
63	 [Boc-L-Phenylalanine][Boc-L-Phenylalanine][Indole-3-acetic acid]	784.0	783.4	N-{(1S)-2-[(anilinocarbonyl)amino]-1-benzylethyl}-N-{(2S)-2-[(anilinocarbonyl)[2-(1H-indol-3-yl)ethyl]amino}-3-phenylpropyl}-N'-phenylurea	4.8	10	5	2
64	 [Boc-L-Phenylalanine][Boc-L-Phenylalanine][3-(3,4,5)-Trimethoxyphenylpropionic acid]	849.0	848.4	N-{(1S)-2-[(anilinocarbonyl)amino]-1-benzylethyl}-N-{(2S)-2-[(anilinocarbonyl)[3-(3,4,5-trimethoxyphenyl)propyl]amino}-3-phenylpropyl}-N'-phenylurea	4.5	12	4	3
65	 [Boc-L-Phenylalanine][Boc-L-Phenylalanine][2-Norbornaneacetic acid]	763.0	762.4	N-{(1S)-2-[(anilinocarbonyl)amino]-1-benzylethyl}-N-{(2S)-2-[(anilinocarbonyl)(2-bicyclo[2.2.1]hept-2-ylethyl)amino}-3-phenylpropyl}-N'-phenylurea	5.7	9	4	2

Figure 22A (cont.)

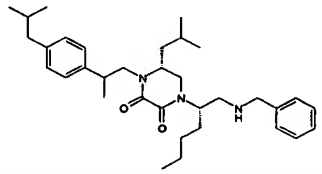
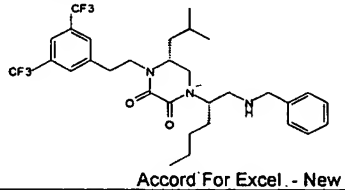
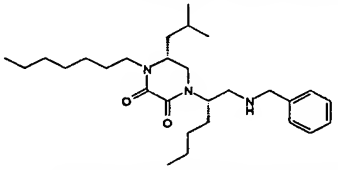
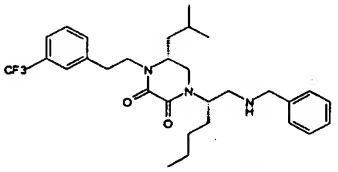
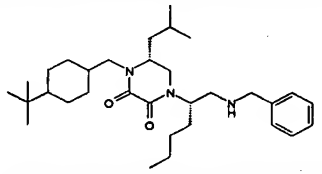
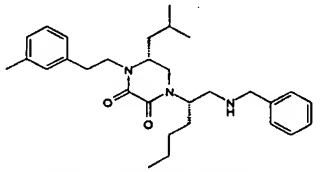
TPI1391	Structures	MW	Exact Mass	Name	M Log P	H Bond Donor	H Bond Donor	Rule Of Five
1	 [Fmoc-L-Norleucine][Fmoc-D-Leucine][4-Isobutyl-alpha-Methylphenylacetic Acid]	533.8	533.4	(5R)-1-{(1S)-1-[(benzylamino)methyl]pentyl}-5-isobutyl-4-[2-(4-isobutylphenyl)propyl]piperazine-2,3-dione	4.6	5	1	2
2	 Accord For Excel - New Chemistry	599.7	599.3	(5R)-1-{(1S)-1-[(benzylamino)methyl]pentyl}-4-{2-[3,5-bis(trifluoromethyl)phenyl]ethyl}-5-isobutylpiperazine-2,3-dione	5.4	5	1	2
3	 [Fmoc-L-Norleucine][Fmoc-D-Leucine][Heptanoic acid]	457.7	457.4	(5R)-1-{(1S)-1-[(benzylamino)methyl]pentyl}-4-heptyl-5-isobutylpiperazine-2,3-dione	3.7	5	1	0
4	 [Fmoc-L-Norleucine][Fmoc-D-Leucine][(Alpha-Alpha-Alpha-Trifluoro-m-Tolyl) acetic acid]	531.7	531.3	(5R)-1-{(1S)-1-[(benzylamino)methyl]pentyl}-5-isobutyl-4-{2-[3-(trifluoromethyl)phenyl]ethyl}piperazine-2,3-dione	4.4	5	1	2
5	 [Fmoc-L-Norleucine][Fmoc-D-Leucine][4-tert-Butyl-cyclohexanecarboxylic acid]	511.8	511.4	(5R)-1-{(1S)-1-[(benzylamino)methyl]pentyl}-4-[(4-tert-butylcyclohexyl)methyl]-5-isobutylpiperazine-2,3-dione	4.5	5	1	2
6	 [Fmoc-L-Norleucine][Fmoc-D-Leucine][m-Tolylacetic acid]	477.7	477.3	(5R)-1-{(1S)-1-[(benzylamino)methyl]pentyl}-5-isobutyl-4-[2-(3-methylphenyl)ethyl]piperazine-2,3-dione	3.9	5	1	0

Figure 23A

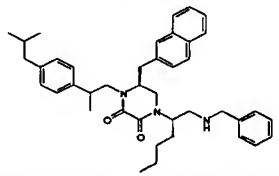
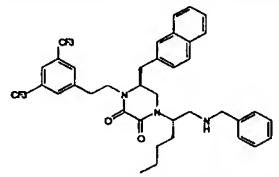
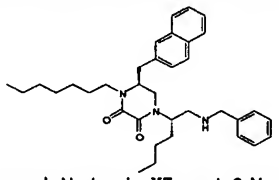
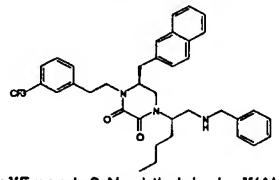
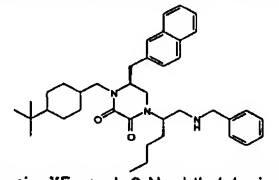
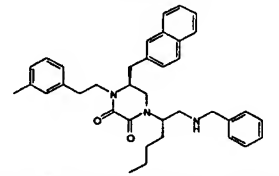
TPI1391	Structures	MW	Exact Mass	Name	M Log P	H Bond Donor	H Bond Donor	Rule Of Five
7	 [Fmoc-L-Norleucine][Fmoc-L-2-Naphthylalanine][4-Isobutyl-alpha-Methylphenylacetic Acid]	617.9	617.4	(5S)-1-{(1S)-1-[(benzylamino)methyl]pentyl}-4-[2-(4-isobutylphenyl)propyl]-5-(2-naphthylmethyl)piperazine-2,3-dione	5.4	5	1	2
8	 [Fmoc-L-Norleucine][Fmoc-L-2-Naphthylalanine][3,5-Bis(Trifluoromethyl)-Phenylacetic Acid]	683.7	683.3	(5S)-1-{(1S)-1-[(benzylamino)methyl]pentyl}-4-{2-[3,5-bis(trifluoromethyl)phenyl]ethyl}-5-(2-naphthylmethyl)piperazine-2,3-dione	6.2	5	1	2
9	 [Fmoc-L-Norleucine][Fmoc-L-2-Naphthylalanine][Heptanoic acid]	541.8	541.4	(5S)-1-{(1S)-1-[(benzylamino)methyl]pentyl}-4-heptyl-5-(2-naphthylmethyl)piperazine-2,3-dione	4.6	5	1	2
10	 moc-L-Norleucine][Fmoc-L-2-Naphthylalanine][(Alpha-Alpha-Alpha-Trifluoro-m-Tolyl) acetic ac	615.7	615.3	(5S)-1-{(1S)-1-[(benzylamino)methyl]pentyl}-5-(2-naphthylmethyl)-4-{2-[3-(trifluoromethyl)phenyl]ethyl}piperazine-2,3-dione	5.3	5	1	2
11	 [Fmoc-L-Norleucine][Fmoc-L-2-Naphthylalanine][4-tert-Butyl-cyclohexanecarboxylic acid]	595.9	595.4	(5S)-1-{(1S)-1-[(benzylamino)methyl]pentyl}-4-[(4-tert-butylcyclohexyl)methyl]-5-(2-naphthylmethyl)piperazine-2,3-dione	5.3	5	1	2
12	 [Fmoc-L-Norleucine][Fmoc-L-2-Naphthylalanine][m-Tolylacetic acid]	561.8	561.3	(5S)-1-{(1S)-1-[(benzylamino)methyl]pentyl}-4-[2-(3-methylphenyl)ethyl]-5-(2-naphthylmethyl)piperazine-2,3-dione	4.7	5	1	2

Figure 23A (cont.)

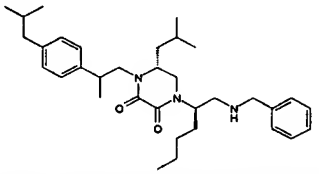
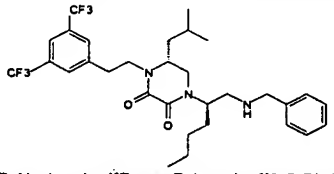
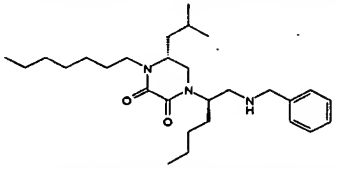
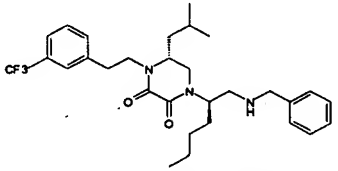
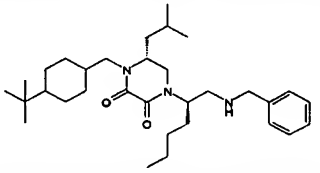
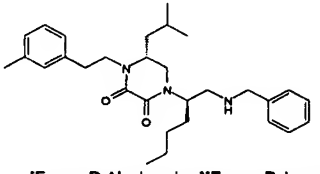
TPI1391	Structures	MW	Exact Mass	Name	M Log P	H Bond Donor	H Bond Donor	Rule Of Five
13	 [Fmoc-D-Norleucine][Fmoc-D-Leucine][4-Isobutyl-alpha-Methylphenylacetic Acid]	533.8	533.4	(5R)-1-{(1R)-1-[(benzylamino)methyl]pentyl}-5-isobutyl-4-[2-(4-isobutylphenyl)propyl]piperazine-2,3-dione	4.6	5	1	2
14	 [Fmoc-D-Norleucine][Fmoc-D-Leucine][3,5-Bis(Trifluoromethyl)-Phenylacetic Acid]	599.7	599.3	(5R)-1-{(1R)-1-[(benzylamino)methyl]pentyl}-4-{2-[3,5-bis(trifluoromethyl)phenyl]ethyl}-5-isobutylpiperazine-2,3-dione	5.4	5	1	2
15	 [Fmoc-D-Norleucine][Fmoc-D-Leucine][Heptanoic acid]	457.7	457.4	(5R)-1-{(1R)-1-[(benzylamino)methyl]pentyl}-4-heptyl-5-isobutylpiperazine-2,3-dione	3.7	5	1	0
16	 [Fmoc-D-Norleucine][Fmoc-D-Leucine][(Alpha-Alpha-Alpha-Trifluoro-m-Tolyl) acetic acid]	531.7	531.3	(5R)-1-{(1R)-1-[(benzylamino)methyl]pentyl}-5-isobutyl-4-{2-[3-(trifluoromethyl)phenyl]ethyl}piperazine-2,3-dione	4.4	5	1	2
17	 [Fmoc-D-Norleucine][Fmoc-D-Leucine][4-tert-Butyl-cyclohexanecarboxylic acid]	511.8	511.4	(5R)-1-{(1R)-1-[(benzylamino)methyl]pentyl}-4-[(4-tert-butylcyclohexyl)methyl]-5-isobutylpiperazine-2,3-dione	4.5	5	1	2
18	 [Fmoc-D-Norleucine][Fmoc-D-Leucine][m-Tolylacetic acid]	477.7	477.3	(5R)-1-{(1R)-1-[(benzylamino)methyl]pentyl}-5-isobutyl-4-[2-(3-methylphenyl)ethyl]piperazine-2,3-dione	3.9	5	1	0

Figure 23A (cont.)

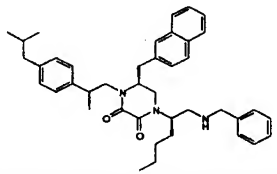
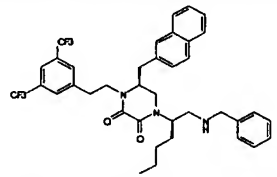
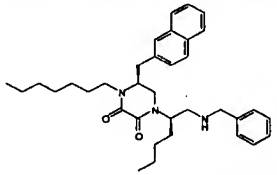
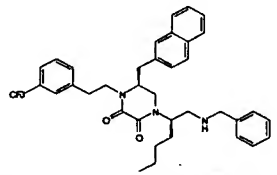
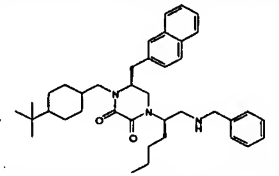
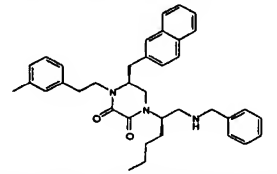
TPI1391	Structures	MW	Exact Mass	Name	M Log P	H Bond Donor	H Bond Donor	Rule Of Five
19	 [Fmoc-D-Norleucine][Fmoc-L-2-Naphthylalanine][4-Isobutyl-alpha-Methylphenylacetic Acid]	617.9	617.4	(5S)-1-{(1R)-1-[(benzylamino)methyl]pentyl}-4-[2-(4-isobutylphenyl)propyl]-5-(2-naphthylmethyl)piperazine-2,3-dione	5.4	5	1	2
20	 [Fmoc-D-Norleucine][Fmoc-L-2-Naphthylalanine][3,5-Bis(Trifluoromethyl)-Phenylacetic Acid]	683.7	683.3	(5S)-1-{(1R)-1-[(benzylamino)methyl]pentyl}-4-{2-[3,5-bis(trifluoromethyl)phenyl]ethyl}-5-(2-naphthylmethyl)piperazine-2,3-dione	6.2	5	1	2
21	 FALSE	541.8	541.4	(5S)-1-{(1R)-1-[(benzylamino)methyl]pentyl}-4-heptyl-5-(2-naphthylmethyl)piperazine-2,3-dione	4.6	5	1	2
22	 moc-D-Norleucine][Fmoc-L-2-Naphthylalanine][(Alpha-Alpha-Alpha-Trifluoro-m-Tolyl) acetic ac	615.7	615.3	(5S)-1-{(1R)-1-[(benzylamino)methyl]pentyl}-5-(2-naphthylmethyl)-4-{2-[3-(trifluoromethyl)phenyl]ethyl}piperazine-2,3-dione	5.3	5	1	2
23	 [Fmoc-D-Norleucine][Fmoc-L-2-Naphthylalanine][4-tert-Butyl-cyclohexanecarboxylic acid]	595.9	595.4	(5S)-1-{(1R)-1-[(benzylamino)methyl]pentyl}-4-[(4-tert-butylcyclohexyl)methyl]-5-(2-naphthylmethyl)piperazine-2,3-dione	5.3	5	1	2
24	 [Fmoc-D-Norleucine][Fmoc-L-2-Naphthylalanine][m-Tolylacetic acid]	561.8	561.3	(5S)-1-{(1R)-1-[(benzylamino)methyl]pentyl}-4-[2-(3-methylphenyl)ethyl]-5-(2-naphthylmethyl)piperazine-2,3-dione	4.7	5	1	2

Figure 23A (cont.)

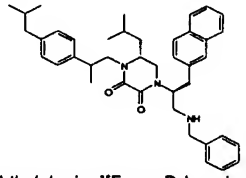
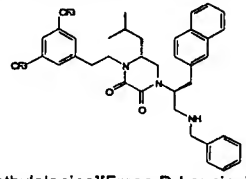
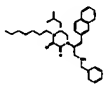
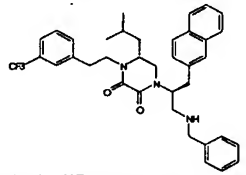
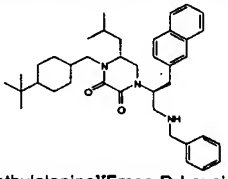
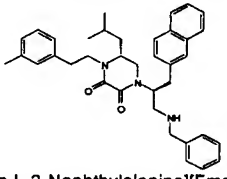
TPI1391	Structures	MW	Exact Mass	Name	M Log P	H Bond Donor	H Bond Donor	Rule Of Five
25	 [Fmoc-L-2-Naphthylalanine][Fmoc-D-Leucine][4-Isobutyl-alpha-Methylphenylacetic Acid]	617.9	617.4	(5R)-1-[(1S)-2-(benzylamino)-1-(2-naphthylmethyl)ethyl]-5-isobutyl-4-[2-(4-isobutylphenyl)propyl]piperazine-2,3-dione	5.4	5	1	2
26	 [Fmoc-L-2-Naphthylalanine][Fmoc-D-Leucine][3,5-Bis(Trifluoromethyl)-Phenylacetic Acid]	683.7	683.3	(5R)-1-[(1S)-2-(benzylamino)-1-(2-naphthylmethyl)ethyl]-4-[2-[3,5-bis(trifluoromethyl)phenyl]ethyl]-5-isobutylpiperazine-2,3-dione	6.2	5	1	2
27	 [Fmoc-L-2-Naphthylalanine][Fmoc-D-Leucine][Heptanoic acid]	541.8	541.4	(5R)-1-[(1S)-2-(benzylamino)-1-(2-naphthylmethyl)ethyl]-4-heptyl-5-isobutylpiperazine-2,3-dione	4.6	5	1	2
28	 Fmoc-L-2-Naphthylalanine][Fmoc-D-Leucine][(Alpha-Alpha-Alpha-Trifluoro-m-Tolyl) acetic acid	615.7	615.3	(5R)-1-[(1S)-2-(benzylamino)-1-(2-naphthylmethyl)ethyl]-5-isobutyl-4-[2-[3-(trifluoromethyl)phenyl]ethyl]piperazine-2,3-dione	5.3	5	1	2
29	 [Fmoc-L-2-Naphthylalanine][Fmoc-D-Leucine][4-tert-Butyl-cyclohexanecarboxylic acid]	595.9	595.4	(5R)-1-[(1S)-2-(benzylamino)-1-(2-naphthylmethyl)ethyl]-4-[(4-tert-butylcyclohexyl)methyl]-5-isobutylpiperazine-2,3-dione	5.3	5	1	2
30	 [Fmoc-L-2-Naphthylalanine][Fmoc-D-Leucine][m-Tolylacetic acid]	561.8	561.3	(5R)-1-[(1S)-2-(benzylamino)-1-(2-naphthylmethyl)ethyl]-5-isobutyl-4-[2-(3-methylphenyl)ethyl]piperazine-2,3-dione	4.7	5	1	2

Figure 23A (cont.)

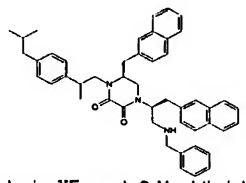
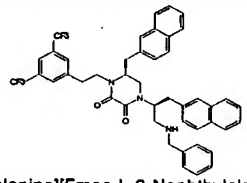
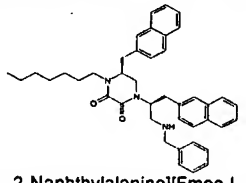
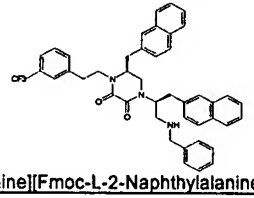
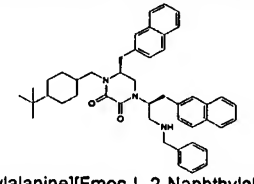
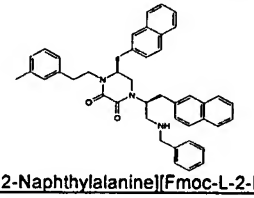
TPI1391	Structures	MW	Exact Mass	Name	M Log P	H Bond Donor	H Bond Donor	Rule Of Five
31	 moc-L-2-Naphthylalanine][Fmoc-L-2-Naphthylalanine][4-Isobutyl-alpha-Methylphenylacetic Aci	702.0	701.4	(5S)-1-[(1S)-2-(benzylamino)-1-(2-naphthylmethyl)ethyl]-4-[2-(4-isobutylphenyl)propyl]-5-(2-naphthylmethyl)piperazine-2,3-dione	6.2	5	1	2
32	 moc-L-2-Naphthylalanine][Fmoc-L-2-Naphthylalanine][3,5-Bis(Trifluoromethyl)-Phenylacetic Ac	767.8	767.3	(5S)-1-[(1S)-2-(benzylamino)-1-(2-naphthylmethyl)ethyl]-4-[2-[3,5-bis(trifluoromethyl)phenyl]ethyl]-5-(2-naphthylmethyl)piperazine-2,3-dione	7.0	5	1	2
33	 [Fmoc-L-2-Naphthylalanine][Fmoc-L-2-Naphthylalanine][Heptanoic acid]	625.9	625.4	(5S)-1-[(1S)-2-(benzylamino)-1-(2-naphthylmethyl)ethyl]-4-heptyl-5-(2-naphthylmethyl)piperazine-2,3-dione	5.4	5	1	2
34	 c-L-2-Naphthylalanine][Fmoc-L-2-Naphthylalanine][(Alpha-Alpha-Alpha-Trifluoro-m-Tolyl) acetic	699.8	699.3	(5S)-1-[(1S)-2-(benzylamino)-1-(2-naphthylmethyl)ethyl]-5-(2-naphthylmethyl)-4-(2-[3-(trifluoromethyl)phenyl]ethyl)piperazine-2,3-dione	6.1	5	1	2
35	 Fmoc-L-2-Naphthylalanine][Fmoc-L-2-Naphthylalanine][4-tert-Butyl-cyclohexanecarboxylic acid	679.9	679.4	(5S)-1-[(1S)-2-(benzylamino)-1-(2-naphthylmethyl)ethyl]-4-[(4-tert-butylcyclohexyl)methyl]-5-(2-naphthylmethyl)piperazine-2,3-dione	6.1	5	1	2
36	 [Fmoc-L-2-Naphthylalanine][Fmoc-L-2-Naphthylalanine][m-Tolylacetic acid]	645.8	645.3	(5S)-1-[(1S)-2-(benzylamino)-1-(2-naphthylmethyl)ethyl]-4-[2-(3-methylphenyl)ethyl]-5-(2-naphthylmethyl)piperazine-2,3-dione	5.6	5	1	2

Figure 23A (cont.)

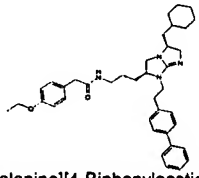
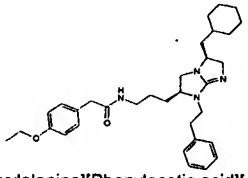
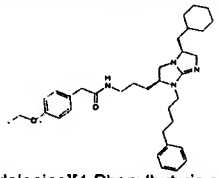
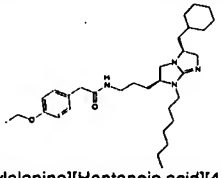
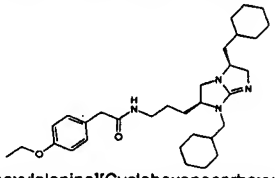
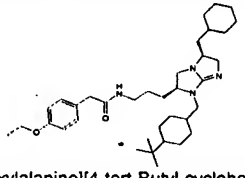
TPI1400	Structures	MW	Exact Mass	Name	M Log P	H Bond Acceptor	H Bond Donor	Rule Of Five
1	 [Boc-L-Cyclohexylalanine][4-Biphenylacetic acid][4-Ethoxyphenylacetic acid]	606.9	606.4	N-{3-[(2S,5S)-1-[2-(1,1'-biphenyl-4-yl)ethyl]-5-(cyclohexylmethyl)-2,3,5,6-tetrahydro-1H-imidazo[1,2-a]imidazol-2-yl]propyl}-2-(4-ethoxyphenyl)acetamide	5.6	6	1	2
2	 [Boc-L-Cyclohexylalanine][Phenylacetic acid][4-Ethoxyphenylacetic acid]	530.8	530.4	N-{3-[(2S,5S)-5-(cyclohexylmethyl)-1-(2-phenylethyl)-2,3,5,6-tetrahydro-1H-imidazo[1,2-a]imidazol-2-yl]propyl}-2-(4-ethoxyphenyl)acetamide	4.7	6	1	2
3	 [Boc-L-Cyclohexylalanine][4-Phenylbutyric acid][4-Ethoxyphenylacetic acid]	558.8	558.4	N-{3-[(2S,5S)-5-(cyclohexylmethyl)-1-(4-phenylbutyl)-2,3,5,6-tetrahydro-1H-imidazo[1,2-a]imidazol-2-yl]propyl}-2-(4-ethoxyphenyl)acetamide	5.1	6	1	2
4	 [Boc-L-Cyclohexylalanine][Heptanoic acid][4-Ethoxyphenylacetic acid]	524.8	524.4	N-{3-[(2S,5S)-5-(cyclohexylmethyl)-1-heptyl-2,3,5,6-tetrahydro-1H-imidazo[1,2-a]imidazol-2-yl]propyl}-2-(4-ethoxyphenyl)acetamide	4.8	6	1	2
5	 [Boc-L-Cyclohexylalanine][Cyclohexanecarboxylic acid][4-Ethoxyphenylacetic acid]	522.8	522.4	N-{3-[(2S,5S)-1,5-bis(cyclohexylmethyl)-2,3,5,6-tetrahydro-1H-imidazo[1,2-a]imidazol-2-yl]propyl}-2-(4-ethoxyphenyl)acetamide	4.8	6	1	2
6	 [Boc-L-Cyclohexylalanine][4-tert-Butyl-cyclohexanecarboxylic acid][4-Ethoxyphenylacetic acid]	578.9	578.5	N-{3-[(2S,5S)-1-[(4-tert-butylcyclohexyl)methyl]-5-(cyclohexylmethyl)-2,3,5,6-tetrahydro-1H-imidazo[1,2-a]imidazol-2-yl]propyl}-2-(4-ethoxyphenyl)acetamide	5.5	6	1	2

Figure 24A

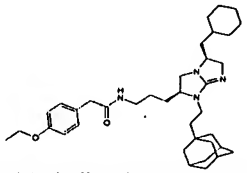
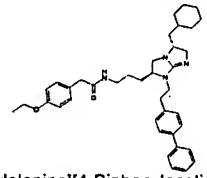
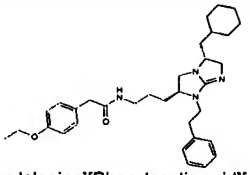
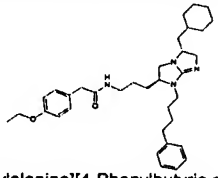
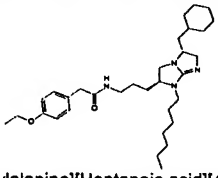
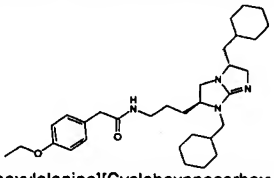
TPI1400	Structures	MW	Exact Mass	Name	M Log P	H Bond Acceptor	H Bond Donor	Rule Of Five
7	 [Boc-L-Cyclohexylalanine][1-Adamantaneacetic acid][4-Ethoxyphenylacetic acid]	588.9	588.4	N-{3-[(2S,5S)-1-[2-(1-adamantyl)ethyl]-5-(cyclohexylmethyl)-2,3,5,6-tetrahydro-1H-imidazo[1,2-a]imidazol-2-yl]propyl}-2-(4-ethoxyphenyl)acetamide	5.7	6	1	2
8	 [Boc-D-Cyclohexylalanine][4-Biphenylacetic acid][4-Ethoxyphenylacetic acid]	606.9	606.4	N-{3-[(2S,5R)-1-[2-(1,1'-biphenyl-4-yl)ethyl]-5-(cyclohexylmethyl)-2,3,5,6-tetrahydro-1H-imidazo[1,2-a]imidazol-2-yl]propyl}-2-(4-ethoxyphenyl)acetamide	5.6	6	1	2
9	 [Boc-D-Cyclohexylalanine][Phenylacetic acid][4-Ethoxyphenylacetic acid]	530.8	530.4	N-{3-[(2S,5R)-5-(cyclohexylmethyl)-1-(2-phenylethyl)-2,3,5,6-tetrahydro-1H-imidazo[1,2-a]imidazol-2-yl]propyl}-2-(4-ethoxyphenyl)acetamide	4.7	6	1	2
10	 [Boc-D-Cyclohexylalanine][4-Phenylbutyric acid][4-Ethoxyphenylacetic acid]	558.8	558.4	N-{3-[(2S,5R)-5-(cyclohexylmethyl)-1-(4-phenylbutyl)-2,3,5,6-tetrahydro-1H-imidazo[1,2-a]imidazol-2-yl]propyl}-2-(4-ethoxyphenyl)acetamide	5.1	6	1	2
11	 [Boc-D-Cyclohexylalanine][Heptanoic acid][4-Ethoxyphenylacetic acid]	524.8	524.4	N-{3-[(2S,5R)-5-(cyclohexylmethyl)-1-heptyl-2,3,5,6-tetrahydro-1H-imidazo[1,2-a]imidazol-2-yl]propyl}-2-(4-ethoxyphenyl)acetamide	4.8	6	1	2
12	 [Boc-D-Cyclohexylalanine][Cyclohexanecarboxylic acid][4-Ethoxyphenylacetic acid]	522.8	522.4	N-{3-[(2S,5R)-1,5-bis(cyclohexylmethyl)-2,3,5,6-tetrahydro-1H-imidazo[1,2-a]imidazol-2-yl]propyl}-2-(4-ethoxyphenyl)acetamide	4.8	6	1	2

Figure 24A (cont.)

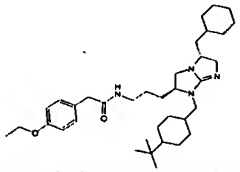
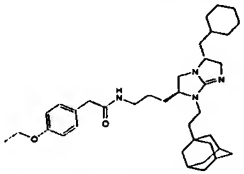
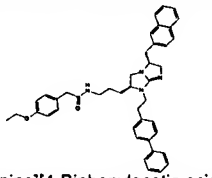
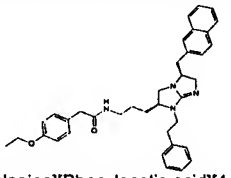
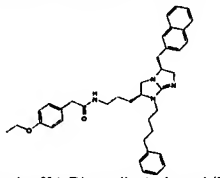
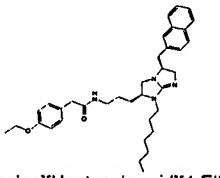
TPI1400	Structures	MW	Exact Mass	Name	M Log P	H Bond Acceptor	H Bond Donor	Rule Of Five
13	 [Boc-D-Cyclohexylalanine][4-tert-Butyl-cyclohexanecarboxylic acid][4-Ethoxyphenylacetic acid]	578.9	578.5	N-{3-[(2S,5R)-1-[(4-tert-butylcyclohexyl)methyl]-5-(cyclohexylmethyl)-2,3,5,6-tetrahydro-1H-imidazo[1,2-a]imidazol-2-yl]propyl}-2-(4-ethoxyphenyl)acetamide	5.5	6	1	2
14	 [Boc-D-Cyclohexylalanine][1-Adamantaneacetic acid][4-Ethoxyphenylacetic acid]	588.9	588.4	N-{3-[(2S,5R)-1-[2-(1-adamantyl)ethyl]-5-(cyclohexylmethyl)-2,3,5,6-tetrahydro-1H-imidazo[1,2-a]imidazol-2-yl]propyl}-2-(4-ethoxyphenyl)acetamide	5.7	6	1	2
15	 [Boc-L-Naphthylalanine][4-Biphenylacetic acid][4-Ethoxyphenylacetic acid]	650.9	650.4	N-{3-[(2S,5S)-1-[2-(1,1'-biphenyl-4-yl)ethyl]-5-(2-naphthylmethyl)-2,3,5,6-tetrahydro-1H-imidazo[1,2-a]imidazol-2-yl]propyl}-2-(4-ethoxyphenyl)acetamide	5.9	6	1	2
16	 [Boc-L-Naphthylalanine][Phenylacetic acid][4-Ethoxyphenylacetic acid]	574.8	574.3	2-(4-ethoxyphenyl)-N-{3-[(2S,5S)-5-(2-naphthylmethyl)-1-(2-phenylethyl)-2,3,5,6-tetrahydro-1H-imidazo[1,2-a]imidazol-2-yl]propyl}acetamide	5.1	6	1	2
17	 [Boc-L-Naphthylalanine][4-Phenylbutyric acid][4-Ethoxyphenylacetic acid]	602.8	602.4	2-(4-ethoxyphenyl)-N-{3-[(2S,5S)-5-(2-naphthylmethyl)-1-(4-phenylbutyl)-2,3,5,6-tetrahydro-1H-imidazo[1,2-a]imidazol-2-yl]propyl}acetamide	5.4	6	1	2
18	 [Boc-L-Naphthylalanine][Heptanoic acid][4-Ethoxyphenylacetic acid]	568.8	568.4	2-(4-ethoxyphenyl)-N-{3-[(2S,5S)-1-heptyl-5-(2-naphthylmethyl)-2,3,5,6-tetrahydro-1H-imidazo[1,2-a]imidazol-2-yl]propyl}acetamide	5.1	6	1	2

Figure 24A (cont.)

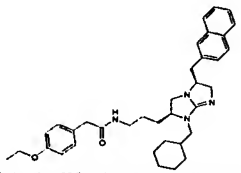
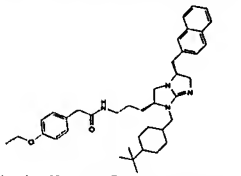
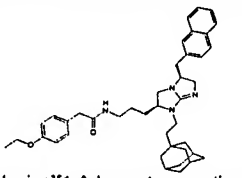
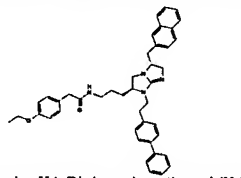
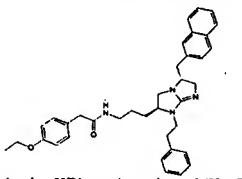
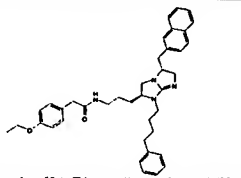
TPI1400	Structures	MW	Exact Mass	Name	M Log P	H Bond Acceptor	H Bond Donor	Rule Of Five
19	 [Boc-L-Naphthylalanine][Cyclohexanecarboxylic acid][4-Ethoxyphenylacetic acid]	566.8	566.4	N-{3-[(2S,5S)-1-(cyclohexylmethyl)-5-(2-naphthylmethyl)-2,3,5,6-tetrahydro-1H-imidazo[1,2-a]imidazol-2-yl]propyl}-2-(4-ethoxyphenyl)acetamide	5.1	6	1	2
20	 [Boc-L-Naphthylalanine][4-tert-Butyl-cyclohexanecarboxylic acid][4-Ethoxyphenylacetic acid]	622.9	622.4	N-{3-[(2S,5S)-1-[(4-tert-butylcyclohexyl)methyl]-5-(2-naphthylmethyl)-2,3,5,6-tetrahydro-1H-imidazo[1,2-a]imidazol-2-yl]propyl}-2-(4-ethoxyphenyl)acetamide	5.8	6	1	2
21	 [Boc-L-Naphthylalanine][1-Adamantaneacetic acid][4-Ethoxyphenylacetic acid]	632.9	632.4	N-{3-[(2S,5S)-1-[2-(1-adamantyl)ethyl]-5-(2-naphthylmethyl)-2,3,5,6-tetrahydro-1H-imidazo[1,2-a]imidazol-2-yl]propyl}-2-(4-ethoxyphenyl)acetamide	6.0	6	1	2
22	 [Boc-D-Naphthylalanine][4-Biphenylacetic acid][4-Ethoxyphenylacetic acid]	650.9	650.4	N-{3-[(2S,5R)-1-[2-(1,1'-biphenyl-4-yl)ethyl]-5-(2-naphthylmethyl)-2,3,5,6-tetrahydro-1H-imidazo[1,2-a]imidazol-2-yl]propyl}-2-(4-ethoxyphenyl)acetamide	5.9	6	1	2
23	 [Boc-D-Naphthylalanine][Phenylacetic acid][4-Ethoxyphenylacetic acid]	574.8	574.3	2-(4-ethoxyphenyl)-N-{3-[(2S,5R)-5-(2-naphthylmethyl)-1-(2-phenylethyl)-2,3,5,6-tetrahydro-1H-imidazo[1,2-a]imidazol-2-yl]propyl}acetamide	5.1	6	1	2
24	 [Boc-D-Naphthylalanine][4-Phenylbutyric acid][4-Ethoxyphenylacetic acid]	602.8	602.4	2-(4-ethoxyphenyl)-N-{3-[(2S,5R)-5-(2-naphthylmethyl)-1-(4-phenylbutyl)-2,3,5,6-tetrahydro-1H-imidazo[1,2-a]imidazol-2-yl]propyl}acetamide	5.4	6	1	2

Figure 24A (cont.)

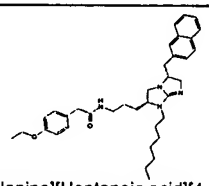
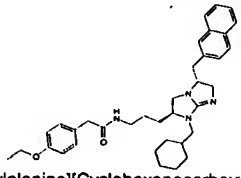
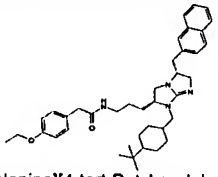
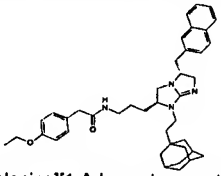
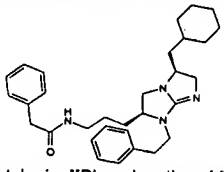
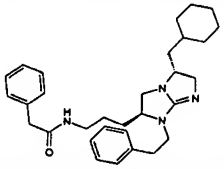
TPI1400	Structures	MW	Exact Mass	Name	M Log P	H Bond Acceptor	H Bond Donor	Rule Of Five
25	 [Boc-D-Naphthylalanine][Heptanoic acid][4-Ethoxyphenylacetic acid]	568.8	568.4	2-(4-ethoxyphenyl)-N-{3-[(2S,5R)-1-heptyl-5-(2-naphthylmethyl)-2,3,5,6-tetrahydro-1H-imidazo[1,2-a]imidazol-2-yl]propyl}acetamide	5.1	6	1	2
26	 [Boc-D-Naphthylalanine][Cyclohexanecarboxylic acid][4-Ethoxyphenylacetic acid]	566.8	566.4	N-{3-[(2S,5R)-1-(cyclohexylmethyl)-5-(2-naphthylmethyl)-2,3,5,6-tetrahydro-1H-imidazo[1,2-a]imidazol-2-yl]propyl}-2-(4-ethoxyphenyl)acetamide	5.1	6	1	2
27	 [Boc-D-Naphthylalanine][4-tert-Butyl-cyclohexanecarboxylic acid][4-Ethoxyphenylacetic acid]	622.9	622.4	N-{3-[(2S,5R)-1-{(4-tert-butylcyclohexyl)methyl}-5-(2-naphthylmethyl)-2,3,5,6-tetrahydro-1H-imidazo[1,2-a]imidazol-2-yl]propyl}-2-(4-ethoxyphenyl)acetamide	5.8	6	1	2
28	 [Boc-D-Naphthylalanine][1-Adamantaneacetic acid][4-Ethoxyphenylacetic acid]	632.9	632.4	N-{3-[(2S,5R)-1-[2-(1-adamantyl)ethyl]-5-(2-naphthylmethyl)-2,3,5,6-tetrahydro-1H-imidazo[1,2-a]imidazol-2-yl]propyl}-2-(4-ethoxyphenyl)acetamide	6.0	6	1	2
29	 [Boc-L-Cyclohexylalanine][Phenylacetic acid][Phenylacetic acid]	486.7	486.3	N-{3-[(2S,5S)-5-(cyclohexylmethyl)-1-(2-phenylethyl)-2,3,5,6-tetrahydro-1H-imidazo[1,2-a]imidazol-2-yl]propyl}-2-phenylacetamide	4.9	5	1	1
30	 [Boc-D-Cyclohexylalanine][Phenylacetic acid][Phenylacetic acid]	486.7	486.3	N-{3-[(2S,5R)-5-(cyclohexylmethyl)-1-(2-phenylethyl)-2,3,5,6-tetrahydro-1H-imidazo[1,2-a]imidazol-2-yl]propyl}-2-phenylacetamide	4.9	5	1	1

Figure 24A (cont.)

TPI1400	Structures	MW	Exact Mass	Name	M Log P	H Bond Acceptor	H Bond Donor	Rule Of Five
31	[Boc-D-p-Chloro-Phenylalanine][Phenylacetic acid][Phenylacetic acid]	515.1	514.2	N-{3-[(2S,5R)-5-(4-chlorobenzyl)-1-(2-phenylethyl)-2,3,5,6-tetrahydro-1H-imidazo[1,2-a]imidazol-2-yl]propyl}-2-phenylacetamide	5.1	5	1	2
32	[Boc-D-p-Fluoro-Phenylalanine][Phenylacetic acid][Phenylacetic acid]	498.6	498.3	N-{3-[(2S,5R)-5-(4-fluorobenzyl)-1-(2-phenylethyl)-2,3,5,6-tetrahydro-1H-imidazo[1,2-a]imidazol-2-yl]propyl}-2-phenylacetamide	5.0	5	1	1
33	[Boc-L-p-Fluoro-Phenylalanine][Phenylacetic acid][Phenylacetic acid]	498.6	498.3	N-{3-[(2S,5S)-5-(4-fluorobenzyl)-1-(2-phenylethyl)-2,3,5,6-tetrahydro-1H-imidazo[1,2-a]imidazol-2-yl]propyl}-2-phenylacetamide	5.0	5	1	1
34	[Boc-D-2-Chloro-Phenylalanine][Phenylacetic acid][Phenylacetic acid]	515.1	514.2	N-{3-[(2S,5R)-5-(2-chlorobenzyl)-1-(2-phenylethyl)-2,3,5,6-tetrahydro-1H-imidazo[1,2-a]imidazol-2-yl]propyl}-2-phenylacetamide	5.1	5	1	2
35	[Boc-L-O-Ethyl-Tyrosine][Phenylacetic acid][Phenylacetic acid]	524.7	524.3	N-{3-[(2S,5S)-5-(4-ethoxybenzyl)-1-(2-phenylethyl)-2,3,5,6-tetrahydro-1H-imidazo[1,2-a]imidazol-2-yl]propyl}-2-phenylacetamide	4.5	6	1	2
36	[Boc-D-O-Ethyl-Tyrosine][Phenylacetic acid][Phenylacetic acid]	524.7	524.3	N-{3-[(2S,5R)-5-(4-ethoxybenzyl)-1-(2-phenylethyl)-2,3,5,6-tetrahydro-1H-imidazo[1,2-a]imidazol-2-yl]propyl}-2-phenylacetamide	4.5	6	1	2

Figure 24A (cont.)

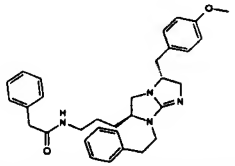
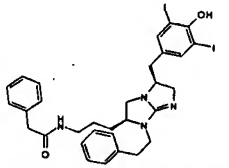
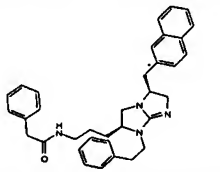
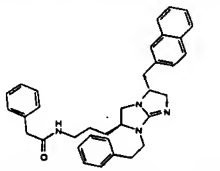
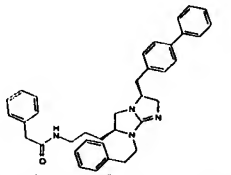
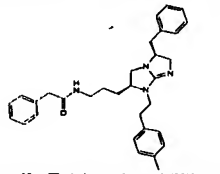
TPI1400	Structures	MW	Exact Mass	Name	M Log P	H Bond Acceptor	H Bond Donor	Rule Of Five
37	 [Boc-D-O-Methyl-Tyrosine][Phenylacetic acid][Phenylacetic acid]	510.7	510.3	N-{3-[(2S,5R)-5-(4-methoxybenzyl)-1-(2-phenylethyl)-2,3,5,6-tetrahydro-1H-imidazo[1,2-a]imidazol-2-yl]propyl}-2-phenylacetamide	4.3	6	1	2
38	 [Boc-L-3,5-Diiodo-Tyrosine(BrZ)][Phenylacetic acid][Phenylacetic acid]	748.4	748.1	N-{3-[(2S,5S)-5-(4-hydroxy-3,5-diiodobenzyl)-1-(2-phenylethyl)-2,3,5,6-tetrahydro-1H-imidazo[1,2-a]imidazol-2-yl]propyl}-2-phenylacetamide	5.4	6	2	2
39	 [Boc-L-Naphthylalanine][Phenylacetic acid][Phenylacetic acid]	530.7	530.3	N-{3-[(2S,5S)-5-(2-naphthylmethyl)-1-(2-phenylethyl)-2,3,5,6-tetrahydro-1H-imidazo[1,2-a]imidazol-2-yl]propyl}-2-phenylacetamide	5.2	5	1	2
40	 [Boc-D-Naphthylalanine][Phenylacetic acid][Phenylacetic acid]	530.7	530.3	N-{3-[(2S,5R)-5-(2-naphthylmethyl)-1-(2-phenylethyl)-2,3,5,6-tetrahydro-1H-imidazo[1,2-a]imidazol-2-yl]propyl}-2-phenylacetamide	5.2	5	1	2
41	 [Boc-L-4,4'-Biphenyl-Alanine][Phenylacetic acid][Phenylacetic acid]	556.8	556.3	N-{3-[(2S,5S)-5-(1,1'-biphenyl-4-ylmethyl)-1-(2-phenylethyl)-2,3,5,6-tetrahydro-1H-imidazo[1,2-a]imidazol-2-yl]propyl}-2-phenylacetamide	5.5	5	1	2
42	 [Boc-L-Phenylalanine][p-Tolylacetic acid][Phenylacetic acid]	494.7	494.3	N-(3-{(2S,5S)-5-benzyl-1-[2-(4-methylphenyl)ethyl]-2,3,5,6-tetrahydro-1H-imidazo[1,2-a]imidazol-2-yl}propyl)-2-phenylacetamide	4.8	5	1	1

Figure 24A (cont.)

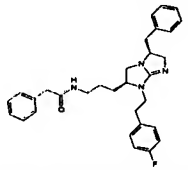
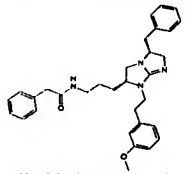
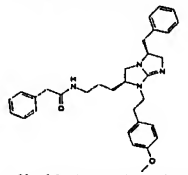
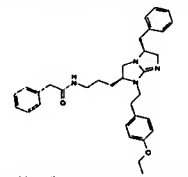
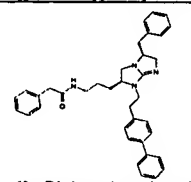
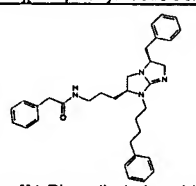
TPI1400	Structures	MW	Exact Mass	Name	M Log P	H Bond Acceptor	H Bond Donor	Rule Of Five
43	 [Boc-L-Phenylalanine][4-Fluorophenylacetic acid][Phenylacetic acid]	498.6	498.3	N-(3-{(2S,5S)-5-benzyl-1-[2-(4-fluorophenyl)ethyl]-2,3,5,6-tetrahydro-1H-imidazo[1,2-a]imidazol-2-yl}propyl)-2-phenylacetamide	5.0	5	1	1
44	 [Boc-L-Phenylalanine][3-Methoxyphenylacetic acid][Phenylacetic acid]	510.7	510.3	N-(3-{(2S,5S)-5-benzyl-1-[2-(3-methoxyphenyl)ethyl]-2,3,5,6-tetrahydro-1H-imidazo[1,2-a]imidazol-2-yl}propyl)-2-phenylacetamide	4.3	6	1	2
45	 [Boc-L-Phenylalanine][4-Methoxyphenylacetic acid][Phenylacetic acid]	510.7	510.3	N-(3-{(2S,5S)-5-benzyl-1-[2-(4-methoxyphenyl)ethyl]-2,3,5,6-tetrahydro-1H-imidazo[1,2-a]imidazol-2-yl}propyl)-2-phenylacetamide	4.3	6	1	2
46	 [Boc-L-Phenylalanine][4-Ethoxyphenylacetic acid][Phenylacetic acid]	524.7	524.3	N-(3-{(2S,5S)-5-benzyl-1-[2-(4-ethoxyphenyl)ethyl]-2,3,5,6-tetrahydro-1H-imidazo[1,2-a]imidazol-2-yl}propyl)-2-phenylacetamide	4.5	6	1	2
47	 [Boc-L-Phenylalanine][4-Biphenylacetic acid][Phenylacetic acid]	556.8	556.3	N-(3-{(2S,5S)-5-benzyl-1-[2-(1,1'-biphenyl-4-yl)ethyl]-2,3,5,6-tetrahydro-1H-imidazo[1,2-a]imidazol-2-yl}propyl)-2-phenylacetamide	5.5	5	1	2
48	 [Boc-L-Phenylalanine][4-Phenylbutyric acid][Phenylacetic acid]	508.7	508.3	N-{3-[(2S,5S)-5-benzyl-1-(4-phenylbutyl)-2,3,5,6-tetrahydro-1H-imidazo[1,2-a]imidazol-2-yl]propyl}-2-phenylacetamide	5.0	5	1	2

Figure 24A (cont.)

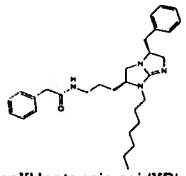
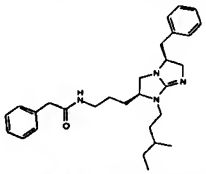
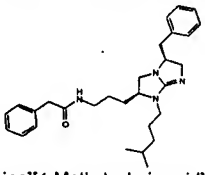
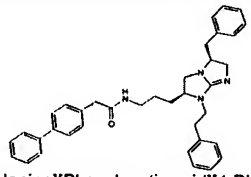
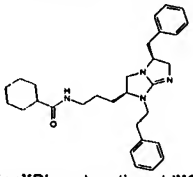
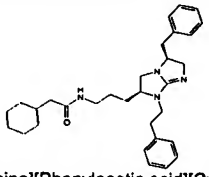
TPI1400	Structures	MW	Exact Mass	Name	M Log P	H Bond Acceptor	H Bond Donor	Rule Of Five
49	 [Boc-L-Phenylalanine][Heptanoic acid][Phenylacetic acid]	474.7	474.3	N-{3-[(2S,5S)-5-benzyl-1-heptyl-2,3,5,6-tetrahydro-1H-imidazo[1,2-a]imidazol-2-yl]propyl}-2-phenylacetamide	4.7	5	1	1
50	 [Boc-L-Phenylalanine][3-Methylvaleric acid][Phenylacetic acid]	460.7	460.3	N-{3-[(2S,5S)-5-benzyl-1-(3-methylpentyl)-2,3,5,6-tetrahydro-1H-imidazo[1,2-a]imidazol-2-yl]propyl}-2-phenylacetamide	4.5	5	1	1
51	 [Boc-L-Phenylalanine][4-Methylvaleric acid][Phenylacetic acid]	460.7	460.3	N-{3-[(2S,5S)-5-benzyl-1-(4-methylpentyl)-2,3,5,6-tetrahydro-1H-imidazo[1,2-a]imidazol-2-yl]propyl}-2-phenylacetamide	4.5	5	1	1
52	 [Boc-L-Phenylalanine][Phenylacetic acid][4-Biphenylacetic acid]	556.8	556.3	N-{3-[(2S,5S)-5-benzyl-1-(2-phenylethyl)-2,3,5,6-tetrahydro-1H-imidazo[1,2-a]imidazol-2-yl]propyl}-2-(1,1'-biphenyl-4-yl)acetamide	5.5	5	1	2
53	 [Boc-L-Phenylalanine][Phenylacetic acid][Cyclohexanecarboxylic acid]	472.7	472.3	N-{3-[(2S,5S)-5-benzyl-1-(2-phenylethyl)-2,3,5,6-tetrahydro-1H-imidazo[1,2-a]imidazol-2-yl]propyl}cyclohexanecarboxamide	4.7	5	1	1
54	 [Boc-L-Phenylalanine][Phenylacetic acid][Cyclohexaneacetic acid]	486.7	486.3	N-{3-[(2S,5S)-5-benzyl-1-(2-phenylethyl)-2,3,5,6-tetrahydro-1H-imidazo[1,2-a]imidazol-2-yl]propyl}-2-cyclohexylacetamide	4.9	5	1	1

Figure 24A (cont.)

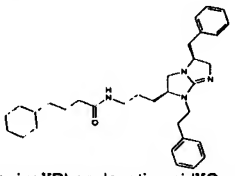
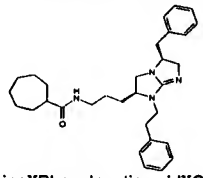
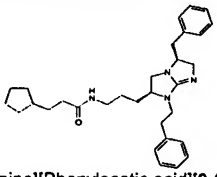
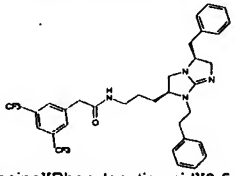
TPI1400	Structures	MW	Exact Mass	Name	M Log P	H Bond Acceptor	H Bond Donor	Rule Of Five
55	 [Boc-L-Phenylalanine][Phenylacetic acid][Cyclohexanebutyric acid]	514.8	514.4	N-{3-[(2S,5S)-5-benzyl-1-(2-phenylethyl)-2,3,5,6-tetrahydro-1H-imidazo[1,2-a]imidazol-2-yl]propyl}-4-cyclohexylbutanamide	5.2	5	1	2
56	 [Boc-L-Phenylalanine][Phenylacetic acid][Cycloheptanecarboxylic acid]	486.7	486.3	N-{3-[(2S,5S)-5-benzyl-1-(2-phenylethyl)-2,3,5,6-tetrahydro-1H-imidazo[1,2-a]imidazol-2-yl]propyl}cycloheptanecarboxamide	4.9	5	1	1
57	 [Boc-L-Phenylalanine][Phenylacetic acid][3-Cyclopentylproplonic acid]	486.7	486.3	N-{3-[(2S,5S)-5-benzyl-1-(2-phenylethyl)-2,3,5,6-tetrahydro-1H-imidazo[1,2-a]imidazol-2-yl]propyl}-3-cyclopentylpropanamide	4.9	5	1	1
58	 [Boc-L-Phenylalanine][Phenylacetic acid][3,5-bis-(Trifluoromethyl)-phenylacetic acid]	616.6	616.3	N-{3-[(2S,5S)-5-benzyl-1-(2-phenylethyl)-2,3,5,6-tetrahydro-1H-imidazo[1,2-a]imidazol-2-yl]propyl}-2-[3,5-bis(trifluoromethyl)phenyl]acetamide	6.4	5	1	2

Figure 24A (cont.)

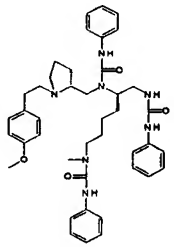
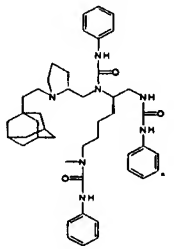
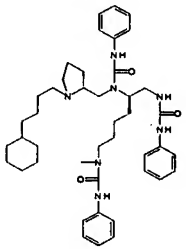
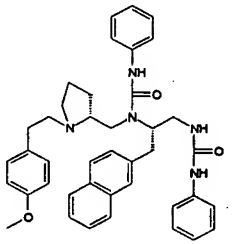
ID #	Name	MW	Structure	Relative caspase 3 activity *		TPI 1396-
				@ 25 ug/ml	[lowest] ug/ml **	L-proline
TPI 1509-1	N-{(5R)-6-[(anilinocarbonyl)amino]-5-[(anilinocarbonyl)({(2R)-1-[2-(4-methoxyphenyl)ethyl]pyrrolidin-2-yl}methyl)amino]hexyl}-N-methyl-N'-phenylurea	719.9		2.2	6.25	10
TPI 1509-2	N-({(2R)-1-[2-(1-adamantyl)ethyl]pyrrolidin-2-yl}methyl)-N-{(1R)-1-{[(anilinocarbonyl)amino]methyl}-5-[(anilinocarbonyl)(methyl)amino]pentyl}-N'-phenylurea	748.0		2.5	12.5	11
TPI 1509-3	N-[(5R)-6-[(anilinocarbonyl)amino]-5-((anilinocarbonyl){[(2R)-1-(4-cyclohexylbutyl)pyrrolidin-2-yl]methyl}amino)hexyl]-N-methyl-N'-phenylurea	724.0		2.4	12.5	12
TPI 1509-4	N-[(1S)-2-[(anilinocarbonyl)amino]-1-(2-naphthylmethyl)ethyl]-N-({(2R)-1-[2-(4-methoxyphenyl)ethyl]pyrrolidin-2-yl}methyl) N'-phenylurea	655.8		2.4	25	22

Figure 34

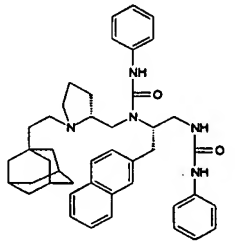
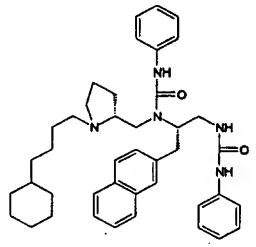
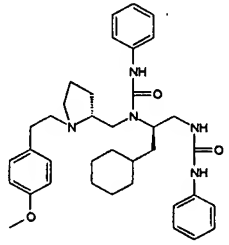
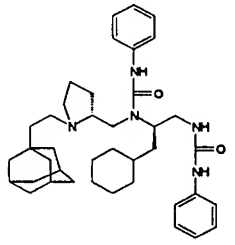
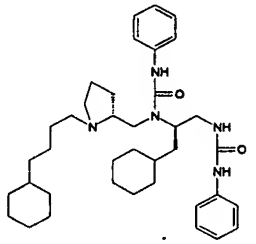
ID #	Name	MW	Structure	@ 25 ug/ml	[lowest] ug/ml **	L-proline
TPI 1509-5	N-({(2R)-1-[2-(1-adamantyl)ethyl]pyrrolidin-2-yl}methyl)-N-[(1S)-2-[(anilinocarbonyl)amino]-1-(2-naphthylmethyl)ethyl]-N'-phenylurea	683.9		2.5	25	23
TPI 1509-6	N-[(1S)-2-[(anilinocarbonyl)amino]-1-(2-naphthylmethyl)ethyl]-N-{[(2R)-1-(4-cyclohexylbutyl)pyrrolidin-2-yl]methyl}-N'-phenylurea	659.9		2.0	12.5	24
TPI 1509-7	N-[(1R)-2-[(anilinocarbonyl)amino]-1-(cyclohexylmethyl)ethyl]-N-({(2R)-1-[2-(4-methoxyphenyl)ethyl]pyrrolidin-2-yl}methyl) N'-phenylurea	611.8		2.4	25	34
TPI 1509-8	N-({(2R)-1-[2-(1-adamantyl)ethyl]pyrrolidin-2-yl}methyl)-N-[(1R)-2-[(anilinocarbonyl)amino]-1-(cyclohexylmethyl)ethyl]-N'-phenylurea	639.9		2.2	25	35

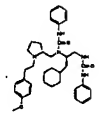
Figure 34 (cont.)

ID #	Name	MW	Structure	@ 25 ug/ml	[lowest] ug/ml **	L-proline
TPI 1509-9	N-[(1R)-2-[(anilinocarbonyl)amino]-1-(cyclohexylmethyl)ethyl]-N-{[(2R)-1-(4-cyclohexylbutyl)pyrrolidin-2-yl]methyl}-N'-phenylurea	615.9		2.2	25	36

Relative caspase-3* activity in the XIAP derepression assay was calculated as the ratio of the Vmax in the presence of each compound divided by the Vmax of the controls ha

[lowest] ug/ml **: lowest concentration in which the relative caspase 3 activity was 1.8

Figure 34 (cont.)



4.26 3 8 2

TPI 1540
Code: 1077
Modifications of TPI1509-7

TPI1509-7 Parent compound
D-Cyclohexylalanine, D-Proline

Lipinski Alerts: MW>500, MlogP > 4.15, HBD>5, HBA>10

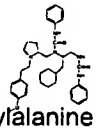
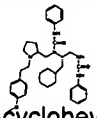
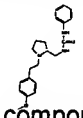
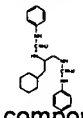
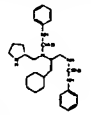
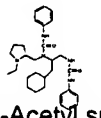
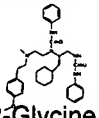
	Structure	MW	Modification	R group	Yield (mg)	MLogP	Hydrogen Bond Donors	Hydrogen Bond Acceptors	Lipinski Alerts
6	 L-cyclohexylalanine analog	611.38	Sterochemistry	R1	54.3	4.26	3	8	2
7	 L-Proline,L-cycloheylalanine analog	611.38	Sterochemistry	R1 and R2	64.4	4.26	3	8	2
8	 Split parent compound-Left side	353.21	Removal of R1 and associated urea	R1	14.8	2.63	2	5	0
9	 Split parent compound-Right side	394.24	Removal of R2 and R3	R2 and R3	32	3.02	4	6	0
10	 Remove R3	477.31	Removal of R3	R3	5.6	3.29	4	7	0
11	 Remove R3-Acetyl substitution (ethyl)	505.3	Replacement of R3 with ethyl	R3	51.1	3.68	3	7	1
12	 Remove R2-Glycine substitution	585.37	Removal of R2	R2	56.1	3.90	3	8	1

Figure 35A

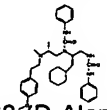
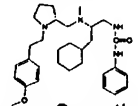
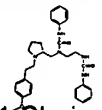
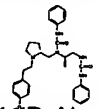
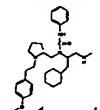
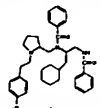
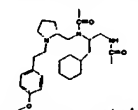
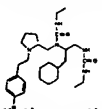
	Structure	MW	Modification	R group	Yield (mg)	MLogP	Hydrogen Bond Donors	Hydrogen Bond Acceptors	Lipinski Alerts
13	 Remove R2-(D-Alanine) substitution	599.38	Replacement of pyrrolidine with N-metylalanine	R2	60.2	4.08	3	8	1
14	 Remove urea 2-methyl substitution	506.36	Removal of N-urea	Urea	48.7	3.89	2	6	1
15	 Remove R1-Glycine substitution	515.2	Removal of R1	R1	51.2	2.97	3	8	1
16	 Remove R1-(D-Alanine) substitution	529.31	Replacement of R1 with methyl	R1	51.5	3.16	3	8	1
17	 Remove urea 1-methyl substitution	506.36	Removal of N'-urea	Urea	10.3	3.89	2	6	1
18	 Remove ureas-benzoyl substitution	581.36	Replacement of phenylurea with **phenylacyl**	Urea	15.2	4.95	1	6	2
19	 Remove ureas-acetylate	457.33	Replacement of phenylurea with **acetyl**	Urea	18.8	3.01	1	6	0
20	 Urea substitution-ethyl isocyanate	515.38	Replacement of phenylurea with **ethylurea**	Urea	53	2.71	3	8	1

Figure 35A (cont.)

	Structure	MW	Modification	R group	Yield (mg)	MLogP	Hydrogen Bond Donors	Hydrogen Bond Acceptors	Lipinski Alerts
21	Urea substitution-4-methylphenylisocyanate	639.41	Replacement of phenylurea with **p-methylphenylurea**	Urea	67.7	4.61	3	8	2
22	Urea substitution-4-fluorophenylisocyanate	647.36	Replacement of phenylurea with **p-fluorophenylurea**	Urea	72.2	4.70	3	8	2
23	Urea substitution-4-nitrophenylisocyanate	701.35	Replacement of phenylurea with **p-nitrophenylurea**	Urea	66.4	4.39	3	14	3

Figure 35A (cont.)

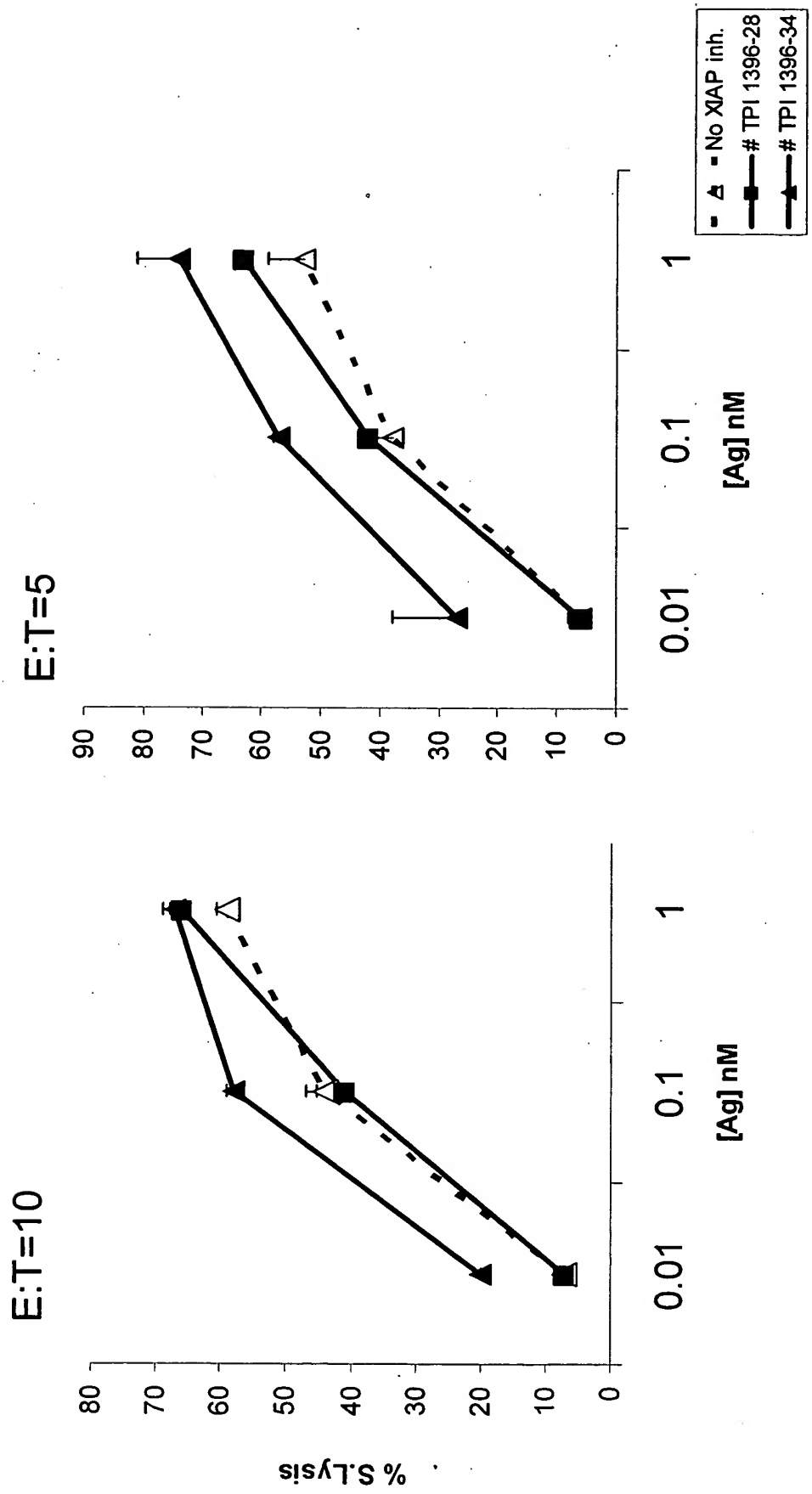

E:T=10
E:T=5
% S.Lysis
[Ag] nM
0.01
0.1
1
0
10
20
30
40
50
60
70
80
90
No XIAP inh.
TPI 1396-28
TPI 1396-34

Figure 39